A XSEDE PD1.3 Project Description

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D Project Description

The **eXtreme Science and Engineering Discovery Environment (XSEDE)** partnership proposes to develop an unprecedented, comprehensive advanced digital services cyberinfrastructure (CI) to enable transformative open science and engineering research and innovative training and educational programs. The goal of XSEDE is to offer users tremendous capabilities with maximum productivity, enabling them to advance and share knowledge across domains. The XSEDE architecture, engineering, operations, support, and education activities are co-designed by an unparalleled team to achieve this goal, far surpassing TeraGrid in usability, reliability, capability, performance, and security—and ultimately, in user productivity and science impact. This proposal and the accompanying supporting documents detail the results of extensive evaluation and planning by the XSEDE team to build this unique cyberinfrastructure.

D.1 Enabling New Digital Science

Computing in science and engineering is now ubiquitous: digital technologies underpin, accelerate, and enable new, even transformational, research in all domains. Informatics and data mining in computational research now complement modeling and simulation. Scientists are now both collecting and generating vast quantities of digital data, introducing new challenges as well as opportunities in the digital science era. Scientists are also increasingly integrating distributed resources and instruments directly into their research and education. The following questions naturally arise: How can we make the impact of diverse, distributed resources greater than what they would have been as stand-alone resources? How can we enable even more transformational science by coordinating, federating, and even integrating these loosely coupled technologies? Is this not especially important for very high-end, relatively rare digital resources? These questions take on greater importance because science is increasingly driven by distributed, collaborating researchers and because data collections emerge from activities conducted worldwide.

Access to an array of integrated and well-supported high-end digital services is critical for the advancement of knowledge in many domains, spanning all directorates of NSF and research supported by other funding agencies (DOE, NIH, DOD, NOAA, etc.). NSF has funded TeraGrid as an HPC-focused CI environment to support diverse research since 2003, while major domain-specific science projects—including the Large Hadron Collider, the Southern California Earthquake Center, the Network for Earthquake Engineering Simulation, the Ocean Observing Infrastructure project, and the iPlant Collaborative—have developed, or are working to develop, integrated CIs for specific research challenges. The NSF Office of Cyberinfrastructure now aims to extend the scope and impact of TeraGrid to offer a more powerful solution: a comprehensive, integrated CI of advanced digital services that enables the next generation of knowledge discovery for important research problems and educational needs spanning domains, campuses, and CI projects.

The **eXtreme Science and Engineering Discovery Environment (XSEDE)** partnership will fulfill this vision by creating *the most advanced, capable, and robust advanced digital cyberinfrastructure in the world*—and supporting it with the most expert and experienced team of CI professionals. XSEDE will accelerate open scientific discovery and enable researchers, educators, and students across disciplines and across campuses to conduct transformational research efforts and innovative education programs. XSEDE will create strong ties with campus personnel spanning technology, workforce development, and policy issues to enhance CI for research and education. The science case for XSEDE is summarized in §D.2 of this proposal and a more detailed justification is provided in the XSEDE Science Case supplementary document (see PD1.2 Science Case).

The NSF workshop report *History & Theory of Infrastructure: Lessons for New Scientific Cyberinfrastructures* [1] described CI thus: "Cyberinfrastructure is the set of organizational practices, technical infrastructure and social norms that collectively provide for the smooth operation of research and education work at a distance. All three are objects of design and engineering; a cyberinfrastructure will fail if any one is ignored." Supporting XSEDE's design is a professional management and systems engineering approach that will ensure continuous and timely improvements all the while respecting robustness and security. The efforts will be connected to user inputs through continuous feedback collection and advisory inputs. The partnership will establish positions and procedures to ensure persistent responsiveness to the requirements of the open science research and education communities—existing, emerging, and future—by inviting leaders in these communities to participate in the partnership's oversight and management. The partnership will also create regular and transparent means for the broader communities to provide input into the evolution of the XSEDE environment and services. Thus, XSEDE will not only transform the conduct of science and the education of current and future generations of science, technology, engineering, and mathematics (STEM) practitioners, but it also will be transformed itself by the communities who are utilizing it for high-impact research and education.

Through extensive planning activities, XSEDE has developed the architecture, user engagement and support, policy structure, on-going user requirements gathering, and evaluation and assessment practices to meet the evolving needs of the open science community. Our standards-based architecture provides maximum opportunity for federating with other advanced CI resources, for campus bridging, and for software development that enhances XSEDE. XSEDE will work closely with the research and education communities to ensure that their science goals are achieved and to provide expert support that enables maximum end-to-end performance and user productivity. XSEDE staff will also work directly with the service providers operating advanced digital services as part of XD (most of whom are already on the XSEDE team) to deploy the technologies necessary to achieve these goals. These activities are described in the Coordination and Management Services activities in §D.4.

Maximum success will often require collaboration with the best computational technologists in the world. The XSEDE team possesses deep expertise in the operation and use of advanced digital resources and will identify and recruit additional experts to ensure researchers maximum opportunity for impact. The Advanced User Support Service section (§D.5) describes the XSEDE team's comprehensive approach.

XSEDE will carry out a multifaceted Training, Education, and Outreach Services (TEOS) program to raise the competency of the present and future scientific community. XSEDE will work proactively with the nation's educational institutions to create a significantly larger and more diverse STEM workforce. TEOS will broaden participation by working with under-represented faculty and students to engage larger numbers of under-represented individuals from among minority-serving and EPSCoR institutions, women, and people with disabilities. TEOS will disseminate best practices, lessons learned, and quality materials and will leverage external partnerships to scale-up successful practices. These activities are described in §D.6.

We will integrate the XD Technology Insertion Service (TIS) activities—already awarded to the XSEDE team—into our continuously advancing CI and will work closely with the Technology Audit Service (TAS) team to ensure that XSEDE can be effectively evaluated and improved. These activities, described in §D.7, will ensure that XSEDE is robust, easy to use, performing as designed, and evolving constantly to meet the growing demands of scientific research and researchers.

The proposal closes with a summary of the qualifications of the XSEDE team for executing this project in §D.8. Advancing science with the most powerful, diverse, and integrated set of advanced digital services ever—and linking that to other CI projects and to campuses and local research infrastructure—is unprecedented. No engineering and technology plan can anticipate all contingencies and future opportunities. Unforeseen user demands and technical complications are inevitable—and indeed will be a welcome consequence of XSEDE's impact on science. The successful realization of NSF's vision for XD will require deep expertise and vast experience, as well as focused and passionate effort. The XSEDE team is uniquely experienced and qualified for this incredible opportunity.

D.2 Science Case

Below we present a summary of the scientific rationale for the XSEDE plan. The full discussion, to which we will often refer, is given in PD1.2 Science Case. We begin with some general arguments, followed by several examples of concrete scientific projects (we could have presented many more) that will be greatly enhanced by the services that XSEDE will provide. We then give examples of how XSEDE's interoperability with other national and international CIs will also advance major science efforts. Finally, we point out that scientific advances are contingent on a very cyber-literate workforce and present the scientific advantages of coordinating Training, Education, and Outreach activities with Advanced User Support efforts. We conclude with some general observations on additional transformational aspects of XSEDE.

Many XSEDE features are designed to enhance user productivity, with the premise that increased productivity leads to more science. Although the borderline is fuzzy, increased productivity is sometimes the difference between a practical project and an impractical one.

D.2.1 General Arguments for XSEDE

XSEDE will be a comprehensive, expertly managed set of high-end digital services, integrated into a general-purpose infrastructure. Thus, XSEDE will be geographically distributed but architecturally and functionally integrated. The scientific motivation for this approach emerges from two fundamental arguments. The first is that scientific advancement across multiple disciplines requires a variety of resources and services and thus the availability of comprehensive CI, composed of heterogeneous digital resources. These requirements are prescribed in many projects and in various domain workshop reports (see PD1.4 Project Execution Plan, §E.2 Science and Education Requirements). The second argument, which is perhaps more subtle but has underpinned NSF's high-end computing programs for over two decades, is that high-end computational science is better served if these capabilities leverage the aggregate expertise of a small number of leading institutions rather than being either fully centralized at a single institution or being fully decentralized. Full centralization leads to less agility in adapting to changing user demands and to a single point of failure for the entire high-end computational science and engineering enterprise. Different sites each offer a unique perspective of human talent to address a particular suite of community needs, whether in architecture, operations, optimization, or the expression of particular algorithms and methodologies. Together, this talent can support a diverse, general community of research and education. For the nation's scientific vitality, it is best to have access to the aggregate expertise and even different leadership philosophies of leading centers of expertise.

However, these two arguments are only part of the justification for XSEDE. For it is only through the support for tight yet flexible integration and interoperability of the resources and services that a growing number of scientific research activities can move forward efficiently and effectively. This is the foundational motivation for XSEDE, which will support "progress toward the resolution of (Grand Challenge) problems…(which) will require *unusual coordination of and collaboration between* [italics added] the diverse communities of researchers." [2]

Among the great strengths of XSEDE, supported by its architectural approach, is XSEDE's campus bridging capability: integrating campus resources into a secure virtual environment. One consistent message from the user community and other stakeholders is that every research team wants its own customizable digital environment for conducting science with a uniform look and feel (see PD3.5 Input Report). The elements of this environment must be dynamically configurable according to their evolving research needs. XSEDE's architecture and engineering approaches will make this possible. Even when bridged to these additional CI resources, XSEDE will provide users and developers the perception of a single system rather than a set of different systems with different administrative domains. Computing and data resources can be accessed from anywhere, in a uniform fashion, with no need to manually copy data around or launch a shell from system to system. Productivity for users utilizing multiple sites will also be greatly enhanced by such XSEDE features as: single sign-on capability extended to support campus credential-based authentication, submission of a single allocation request with a single review committee for all XD services and resources, a single name space for files, and end-to-end tuning to enable the rapid transfer of data from one site to another. XSEDE will also make it easier for researchers to migrate jobs from heavily used systems to those with more availability. This relies on XSEDE's greater integration of data handling and improved standardization of user interfaces. The lowering of usability barriers will facilitate new communities' incorporating high-end digital resources into their regular work environment and will unleash new developments in science that these communities cannot yet articulate.

D.2.2 Science Requires Comprehensive Cyberinfrastructure Capabilities

In this section, we give brief descriptions of several examples of the challenging projects scientists expect to carry out during the next five or more years, and call out (*in italics*) those features of XSEDE that will facilitate this work. More examples and greater detail are to be found in PD1.2 Science Case.

Earthquake Science Coupled to Civil Engineering: The Southern California Earthquake Center (SCEC) aims to calculate more than 10,000 seismic hazard curves to cover all of southern California, where each calculation requires executing two workflows. One workflow controls several large parallel jobs, while the second comprises about 840,000 short loosely coupled jobs. Their research program over the coming years poses a new significant petascale capability computing and data management and analysis challenge: to be relevant to civil engineering disaster planning and mitigation efforts, they must investigate complex frictional processes on fault surfaces during ruptures with simulations that span physical scales from rock particles (< 1m) to the dimensions of large faults (> 500km) and determine earth structural characteristics from ensembles of such petascale runs. These geophysical models will be coupled to large-scale civil engineering, social, and behavioral models that are required to plan and execute an adequate response to a significant earthquake in California. *Efficient data motion, automated workflows, single name space, and the ability to seamlessly harness both parallel and high-throughput computing are indispensable for this grand challenge*. See also XSEDE's interoperability with Open Science Grid (OSG) below.

Molecular Dynamics: Many researchers (e.g. Voth (Chicago), Schulten (Illinois), Cheatham (Utah)) apply atomistic and coarse-grained molecular dynamics simulation methods to facilitate drug discovery, to perform advanced materials research, to design and understand biomolecular and designed catalysts, and to provide fundamental insight into molecular structure, dynamics, and interactions. Although realistic simulations can be run in days to weeks, their analysis often requires months to years. Hierarchical, loosely and tightly coupled sets of simulations are run simultaneously, adding to the workflow and data management requirements. Progress in this field depends on *access to a diverse set of computational resources, large-scale storage, and rapid data transfer for sophisticated analysis and visualization. It also requires software tools that facilitate workflow management for dynamically monitoring, starting, and stopping of ensemble elements and policies for longer-term data storage*.

Computational Molecular Sciences: Computational chemistry, biochemistry, and material sciences consume the largest proportion of allocations in TeraGrid and may continue to do so in XSEDE. Fields such as mechanical engineering and geology now have the potential to understand cause and effects at a molecular level. This has created a need for Science Gateways such as GridChem [3], which enables quantum chemistry, molecular mechanics and dynamics, and quantum Monte Carlo simulations for molecular, periodic, and solid state systems. Several levels of theory, with increasing computational complexity, exist in each category. Experimentalists use GridChem to validate their experimental spectra or suggest models for unknown compounds or to decipher mechanistic details of reactions. GridChem launches the software packages (Gaussian, MolPro, ADF, Castep, DMol3, NWChem, GAMESS, Aces3, QMCPack, Amber, CHARMM) on those machines at TeraGrid and campus sites that are best suited and most available for the complexity of the problem specified by each end-user. *The continued expansion of such efforts depends on XSEDE's standards-based architecture for job and data management and expertise in designing and building community portals and the work and data flows that connect them to the most appropriate resources.*

Nanotechnology: The Nanoelectronic Modeling Group at Purdue designs microprocessors and other devices when their component sizes dip into the nanoscale. This requires a quantum-mechanical description to capture atomic-scale properties. This team plans and executes their virtual experiments on a variety of resources that must be coordinated to easily transfer data between systems. They have built the NanoHUB Science Gateway, which allows thousands of researchers, educators, and students to easily use modeling and simulation tools. As the accuracy of the models increases and their computational and data processing requirements reach the petascale, *managing the work and data flows for the group's own research and for thousands of NanoHUB end-users will benefit from interoperability of XD's computational resources with Open Science Grid and other sources of high-throughput cycles.*

Plant Science: The iPlant Collaborative is a large-scale CI effort to advance scientific understanding of plants to help provide a safe and sustainable food supply in the face of climate change and to explore potential benefits in renewable energy, medicine, etc. Modern plant biology is a largely data-driven science and by its nature a distributed, collaborative process. Data are collected around the world in hundreds of labs and are stored online in dozens of distributed databases. A major challenge is Quantitative Trait Locus (QTL) mapping in maize, which can lead to the holy grail of crop design: accurate prediction of traits (e.g. drought tolerance) based on genetic sequence. QTL mapping for maize requires more computational capability than is available today, *as well as high-speed access to a variety of genotypic and phenotypic databases distributed at several sites*. As in all data-intensive projects, "ideas and work practices that view data as a fundamentally collective, shared resource, rather than as the private possession of individuals and work groups, could have enormous impact." [1]

Storm Prediction: The Center for the Analysis and Prediction of Storms (CAPS) at the University of Oklahoma plans to achieve forecasts for the entire continental U.S. at 2-4 km resolution, assimilating all data from the national Doppler radar network. This will require continuous access to the computational capability of at least 50,000 Cray XT5 cores and about 50 TB of scratch disk space. About 20 TB of forecast products each day will need to be archived in a repository and made available to many collaborating research institutions, government agencies, and downstream users. 50-100 GB of these data must be sent to the NOAA Hazardous Weather Testbed on the University of Oklahoma campus for real-time analysis and display. CAPS will enable on-demand launching of forecasts from a variety of clients, including mobile devices (phones) in the field, as well as students participating in classroom competitions to predict weather conditions. *Work and data flows that will be sufficiently reliable and capable to sustain this forecast system will require XSEDE's standards-based CI architecture and operational and user support expertise. The architecture also supports pre-emptive scheduling. As part of XSEDE's campus bridging, our network plan will support dynamic provisioning of network resources to assure quality of service and dedicated bandwidth to users whose local networks allow them to take advantage of such capability*.

Epidemiology: The NIH Models for Infectious Disease Agent Studies (MIDAS) National Center of Excellence at the University of Pittsburgh uses agent models of census-based U.S. populations to simulate pandemic spread and to create a virtual laboratory where policy decisions such as school closure, vaccine deployment, and quarantine can be explored. While national scale models will require sustained-petaflop computational performance, this is a data-driven process that *requires a reliable and secure infrastructure for distributed data management, transfer, and role-based access by a wide variety of stakeholders. Analysis, collaboration, and decision support user interfaces and tools need to be provided at the technical and executive level appropriate to public health scientists, government decision makers, and the public. This calls for the open, extensible architecture and the reliable and secure data movement and collaboration tools that XSEDE will provide.*

Brain Science: Reconstructing the complete wiring diagram of an organism at full synaptic resolution is the goal of the emerging field called "connectomics." By 2015, researchers in this field hope to be able to capture, process, and analyze ~1 mm^3 of brain tissue. The corresponding raw data will total at least 6 PB, which will need to be securely archived as well as streamed at ~1 GB/s to a processing system that will align image data for analysis. This will result in ~3 PB of co-registered data. *Many research groups will then want to access the resulting image data repository to conduct analysis and visualization specific to their projects. This will be enabled by XSEDE's data motion, network tuning, and campus bridging.*

Particle Physics: The Large Hadron Collider (LHC) experiments at CERN aim to discover the Higgs boson as well as new physics beyond the current "Standard Model." Experimental data will be shipped around the world via workflows enabling massive data analysis largely through loosely coupled systems, each examining events one at a time. Some experimenters, such as the ATLAS detector team, envision using XD resources for their largest-scale maximum likelihood analyses. Moreover, the experimental results can only be interpreted by comparing them with the predictions of the Standard Model, many of which are computed using lattice Quantum Chromodynamics (LQCD). Thus, *distributed storage systems and data movements need to be organized and orchestrated to support these computational simulations and data analyses across XD and several other CIs. XSEDE will enable the necessary workflows and reliable file transfer, including a coordinated archival approach to assure persistence of important datasets beyond the lifetime of particular resources and service providers.*

Analysis of Large Cosmology Simulations: Analyses of large cosmology datasets, ranging from tens of terabytes to petabytes, need to simultaneously access a single snapshot for quasar identification, generation of galaxy catalogs, etc., or they need access to pairs of snapshots for visualization and time-series analysis. These tasks are well suited to XD systems specializing in data-intensive analysis. The simulations that generate the data require petascale systems. A state of the art computation conducted in 2010 by DiMatteo (Carnegie Mellon) of ~33 billion particles of dark matter and gas in a 0.125 GPc^3 simulation volume required 98,304 cores of *Kraken* (Cray XT5) and produced snapshots of 3-4 TB each. *Moving such output to the XD data machines with large shared memories will enable effective analysis of single snapshots and correlations between pairs of snapshots; subsets of the data need to be staged to researchers' labs on campus. XSEDE data motion and campus bridging capabilities will be essential.*

International Collaboration in Cosmology: The Lambda Cold Dark Matter Model (LCDM) is, in its basics, agreed upon by most professional investigators. But the hard tests of the model that would consider variants of the basic paradigm require large-scale computations in the extremely non-linear domain. These must be multiscale and involve multiple levels of physical input. Effective use of the computational output and comparison with observations will require unprecedented levels of data storage, distribution, and analysis. Since the current strongly competing groups are located in several countries and are using codes based on different numerical methods and on different physical modeling, the effort must be international in scope to be effective and credible. *XSEDE's interoperability with international CIs will help teams attacking similar problems by different methods to share, compare, and analyze each other's methods, data, and conclusions*.

International Collaboration in Plasma Physics: An important goal for the Magnetic Fusion Energy Science (MFES) international research effort is to discover important new plasma phenomena with associated understanding that emerges upon integration of multiple coupled physical processes. The associated computational challenge is to deliver a suite of predictive integrated MFES simulation capabilities that are properly validated against experiments in regimes relevant for producing practical fusion energy. This requires coordinating the efforts of the fusion communities in many different countries. *A program of international collaborations is required to clarify and keep current the science development roadmaps including promising future approaches to software and associated computational cyberinfrastructure, dealing with data management challenges involving preparation of input, workflows for advanced simulations, delivery of results and their verification, uncertainty quantification, and experimental validation. Long-term data preservation and strategies for dealing with changes in storage hardware and software must be taken into account.*

Data-Driven Science: Major data-driven projects, such as LSST, LIGO, and NEES, have developed their own CIs, in order to achieve their scientific aims. In TeraGrid, we have worked with, and learned important lessons from, the Neutron Science Gateway at ORNL. In each of these projects, datasets are derived and collected from experiments, observations, and/or computational campaigns. These collections are maintained either locally, centrally at large centers, or in a decentralized collection management system. Analysis, visualizations, subsequent computation, and other data synthesis operations are conducted on the data to produce final science products such as scholarly publications or online network-accessible databases. Each project has some, often significant, local CI resources. Often, a high profile subset of their applications could benefit from migration to extremely large-scale execution environments at XSEDE Service Provider locations. The requirements for XSEDE are: *1) the ability to provide large-scale computational and data resources as needed; 2) the ability to facilitate large, rapid data transfer between data collection sites and XSEDE resources; and 3) compatible software infrastructures in order to minimize the software modifications required to deploy analyses and computations on XSEDE resources*. This third requirement is often the most difficult since large science projects usually have their own approach that may or may not be compatible with national scale CI efforts. *XSEDE, by adhering to standards-based interfaces, rather than adopting a software stack defined by specific versions of specific packages, will ease this problem.*

D.2.3 Interaction with other National and International Cyberinfrastructures

SCEC and the particle physics community (see above) are excellent examples of groups that require the use of both XSEDE and Open Science Grid (OSG) to maximize their scientific productivity. XSEDE has reached out to OSG with its focus on high-throughput computing. As part of our planning activities, the XSEDE team has already demonstrated a prototype mechanism by which XSEDE jobs can be sent to a Condor system, and by which Condor jobs (and DAGMAN graphs) can be executed with XSEDE (standards-based) interfaces. *XSEDE will enable these national-scale, heterogeneous work and data flows by means of its standards-based architecture featuring single name space and efficient and reliable file transfer*. To further facilitate this, we have developed an agreement with OSG to establish them as a partner with the XSEDE project to provide the high throughput computing resources in which they specialize (see PD2.3 Letters of Commitment). This allows us to provide a more comprehensive CI and to further develop the distributed CI ecosystem.

XSEDE has been working with the Distributed European Infrastructure for Supercomputing Applications (DEISA) [4], which enables Grand Challenges like the cosmology and plasma physics examples described above. By *adopting standards-compliant software implementations like UNICORE 6, the XSEDE architecture greatly facilitates interoperability*. Technical collaboration in exploring common authentication, job submission, and data transfer has already begun. Beyond architecture, some of the recommendations from a joint workshop including XSEDE and DEISA management as well as leading scientists from the US and Europe are: formal set-asides of resource allocations on both CIs for proposals that have participants from both sides; an international summer school, alternating between U.S. and Europe; leverage of user support expertise from both continents in the advanced user support programs; consideration of mirroring each other's data (making this an allocable resource in joint proposals); and common pointers to relevant datasets in various fields.

XSEDE has also reached an agreement with the European Grid Infrastructure (EGI) (see PD2.3 Letters of Commitment), established in 2010, to "create and maintain a pan-European Grid Infrastructure…to guarantee the long-term availability of a generic e-infrastructure for all European research communities and their international collaborators." [5] Technical discussions on working towards standards-based interoperability between XSEDE and EGI have already begun.

D.2.4 User Support, Training, Education, and Outreach

The progress of science depends on developing, training, and assisting scientists to make best use of the rapidly changing CI resources in the NSF program. That is part of the mission of TEOS (§D.6) and AUSS (§D.5). The centralization of these efforts enables the most appropriate experts to be brought to bear to assist users, no matter where the experts are located. That centralization also enables cross-pollination between disciplines and resources. We have often seen examples (see PD1.2 Science Case) of advanced user support professionals transmitting advances and insights at the algorithmic, numerical, coding, and optimization levels between fields of application and between computing systems. *By merging the highly experienced advanced support groups from the four core centers with experts from the other SPs into a* *single team under state-of-the-art project management and systems engineering methods, XSEDE AUSS will ensure that such knowledge transfer takes place with unprecedented scope and efficiency.*

D.2.5 Additional Transformative Effects of XSEDE

Over and above increasing user productivity and enabling new modalities of science, XSEDE will be transformative in sociological ways. It will transform how HPC software is developed, how campuses interact with each other, and how distributed teams collaborate to advance scientific discovery.

The persistence of experts in code development and optimization will transform how HPC software will be developed. By taking advantage of TEOS training and interaction with AUSS personnel, graduate students can achieve proficiency in writing codes. But their focus is primarily on their particular research problem and not on creating robust, maintainable software. As a result, developers of large application packages will be turning to the experts in XSEDE for continued development (this is part of the motivation for OCI's recently developed Software Infrastructure for Sustained Innovation (SI^2) program). By providing a persistent career path, XSEDE can retain experts that individual projects cannot.

By adopting standards-based implementations of CI software, campuses will be able to interact more seamlessly with XSEDE. In addition, they will be able to interact *with each other* by leveraging the XSEDE distributed infrastructure. XSEDE will provide the infrastructure for distributed research teams with their own resources to share them among themselves in a pool that may or may not include XSEDE resources. Increasing inter-university collaboration capability will be truly transformative to the research enterprise. In this case, XSEDE is acting as a catalyst for such interoperability.

The Service Providers provide the heavy-lifting computational, visualization, and storage resources, and XSEDE will improve the ease-of-use and productivity of these resources. As XSEDE succeeds, end-users' attention will move increasingly from working with the infrastructure and resources to working with each other supported by the infrastructure and resources. Their ability to discover transformative knowledge in distributed collaborative teams will be significantly enhanced by access to the comprehensive, seamless CI engineered by XSEDE.

D.3 User Experience

XSEDE will ensure that every user team experiences a customizable work environment that can put the required information and execution resources at their fingertips in the manner that they themselves deem most conducive to their knowledge discovery processes. In the following, we provide examples to illustrate how researchers and educators will become more productive in carrying out the tasks they regularly undertake by virtue of the engineered features of XSEDE architecture and services.

For **experienced users** of TeraGrid Phase II, the productivity boosts will begin at the *information discovery* stage. The XSEDE User Portal (XUP) will enable fast queries to the *information services*, which will contain detailed, current, and reliable descriptions of the hardware, software, and service resources managed by XSEDE. It will also contain information on the *campus bridging* and *science gateway* resources whose owners will opt to have them listed as part of their affiliation with XSEDE. The integrated nature of the XUP will make it easy to query documentation and tutorials that may be needed for the user to decide what to request for their next allocation period. This allocation request will be written and submitted via the XUP to minimize the user's burden and wait time. Once allocated, the users will be able to launch activities ranging from traditional compute jobs to complex, automated work and/or data flows across all XSEDE and affiliated resources from the XUP. They will also have access to efficient client tools allowing them to directly access individual resources in a secure manner from a variety of fixed and mobile clients. Role-based authentication to the XUP will allow the Principal Investigator—and his/her delegate—to add and remove users from her grant and to monitor all aspects of resource consumption, while other users will be able to monitor the resources assigned to their particular tasks. The XUP will also enable users to report problems to the unified XSEDE helpdesk and to interact with the user consultants assigned to help them. The user forums provided in the XUP will also enable users to help each other, by sharing their experiences and expertise with the XSEDE community. Users who collaborate with XSEDE AUSS staff will have access to project-specific areas of the XUP.

Users who wish to adopt automated workflow and data flow technologies for increasingly complex, distributed computing, storage, and visualization systems will greatly benefit from XSEDE. We will provide a standard implementation of each of these capabilities, but users will be able to plug in other standards-conforming solutions of their choice. Applications that depend on multiple systems being able to "see" the same dataset will take advantage of the XSEDE-wide file system that will span service provider sites. The XSEDE Global Federated File System (GFFS) extends beyond the SPs into campus IT centers, research labs and machines, and other standards-compliant grid infrastructures. This will empower users and their applications to access remote resources as if they were local files and directories. By encompassing hierarchical filesystems along with an archival storage replication framework, we will enable a coordinated archival approach to assure persistence of important datasets beyond the lifetime of particular service providers. The XSEDE architecture includes in its foundational layer the mechanisms to support fault-detection and recovery implementations, providing clear, timely, and consistent information to users and workflow engines on what is going on in their application. This will allow rapid, accurate, and actionable troubleshooting when failures do occur. XSEDE will provide the information, tools, training, and expert support necessary for building and maintaining science gateways, workflow software, data repositories, and distributed data management and analysis solutions.

Members of a campus community, having attended a talk by a XSEDE outreach team member, will find a full range of services and facilities designed to help them follow up. Complementing the documentation and training materials that will be at the prospective users' fingertips via the XSEDE User Portal, the outreach team will be eager, if appropriate, to put them in touch with the AUSS Novel and Innovative Projects team who will engage in discussions aimed at developing specific projects to use the most appropriate XD resources, in conjunction with their campus resources and work environment. Such projects will be greatly facilitated by XSEDE's *campus bridging capabilities*. Its homogenous access layer provides the means for users and applications developers to access XSEDE resources in a consistent, user-and-task-appropriate, stable-over-time manner. This means that both the new end-users (who only wish to do their domain science) and their more advanced colleagues (who will develop applications in collaboration with AUSS staff) can work efficiently according to their respective roles. The XSEDE GFFS, along with every other element of the standards-based XSEDE architecture, is designed to reach beyond the SPs to include data resources (files, directory trees, relational databases, instrument data, and community collections), compute resources (clusters, desktops, queues, brokers, or virtual machine images), and security resources that may be located in campus IT centers, in research labs and classrooms, and on fixed and mobile workstations.

D.4 Coordination and Management Service

The XD solicitation discusses the need for a Coordination and Management Service (CMS) to provide the integrative management, software, and operations that are required for an integrated virtual organization comprising distinct, distributed service providers. The TeraGrid Grid Integration Group (GIG) illustrates both the value of such central services and the need for even more coordination and management activity—as articulated in the solicitation. In this section, we present the XSEDE plans for not only management, software, and operations but for some important innovations that will make XSEDE far more capable and productive than TeraGrid. We begin by discussing the XSEDE architecture—a missing element of TeraGrid but fundamentally important to achieving the XD vision and the XSEDE goals.

D.4.1 XSEDE Architecture

The purpose of the XSEDE architecture is to provide an extensible framework that enables diverse services, tools, and processes to be integrated, enabling transformative computational research in a variety of disciplines. XSEDE will provide a national CI with relevant, flexible, and easy-to-use interaction paradigms appropriate for its diverse user communities, from current HPC/Unix experts to domain scientists and students accessing community applications via science gateways and desktop clients. XSEDE will span CIs worldwide and incorporate campus centers as well as national, corporate, and individual research laboratories. The combination of unprecedented accessibility, usability, and shareability will empower scientists in all disciplines to be more productive as they conduct sophisticated, collaborative, large-scale computational research. Achieving these characteristics concurrently requires a carefully designed architecture, not an *ad hoc* software stack.

In the following subsections, we first highlight the functional aspects of the XSEDE architecture, particularly in reference to targeted improvements XSEDE offers relative to current practices. Next, we provide an overview of the *XSEDE System* (XSYS) layered grid architecture. Note that this is a very high level view; for a complete description, see PD3.2 XSEDE Architecture. Lastly, we introduce the XSEDE implementation design, together with results of prototype deployments demonstrating the feasibility of the XSEDE approach in production environments.

D.4.1.1 Functional Highlights of XSEDE

XSEDE will employ the best current practices to introduce new and improved functionalities to enhance the productivity of computational science users. Functional highlights of XSEDE include:

Individualized User Experience. Different users have different requirements and preferences regarding how they interact with computational resources. XSEDE aims to customize the user experience, so that every user can more efficiently and effectively generate science. Every user, whether they need traditional HPC access, complex workflows through a science gateway, or are a new user in a non-traditional field from a partner campus, will select the features of XSYS that are consistent, reliable, and best serve their individual preferences, technical capabilities, and requirements for user control.

XSEDE preserves traditional user access interfaces, while improving the consistency of the environment among XSEDE computational resources and extending access to XSYS grid services to the command-line and to user-developed applications. The XSYS grid architecture provides abstracted interfaces and services for consistent, standardized access to XSEDE resources, facilitating science gateway development and mediated access to computational applications and data by domain scientists. XSYS services also extend accessibility of XSEDE computation and data resources to users' local environments and systems, facilitating greater interaction among XSEDE's and users' local resources. For science gateways (e.g., the nanotechnology, storm prediction, and molecular science examples in the science case), this allows both the developers (who are computing experts) and the end-users (who only wish to do their domain science) to work efficiently in their respective roles.

Enduring Interfaces. The XSEDE team recognizes the importance of providing users with reliable software interfaces that do not change frequently, and that, when they change, minimize impact on users and re-coding burden for developers. The XSYS layers insulate users and applications from changes in the underlying services and resources by providing robust, standard interfaces that will change only as necessary and gradually over time in a well-planned manner. Underlying implementations will be flexible to ensure maximum performance and to permit interfaces to evolve and be extended along with the changing needs of the science community. This is essential particularly for long-running projects with a code base built up over many years, such as the earthquake engineering, particle physics, molecular dynamics, and cosmology projects discussed earlier.

Extending Data Capabilities. XSEDE introduces two data technologies that will improve file sharing, data mobility, and data access over current manual practices of copying files from site to site and ensuring consistency. We call these systems the XSEDE-Wide File System (XWFS) and the Global Federated File System (GFFS) (see PD3.2 XSEDE Architecture, §D.1.2 Data and Metadata and PD3.2 XSEDE Architecture, §D.2.1 Global Federated File System).

The XWFS will span XSEDE Service Provider sites using WAN implementations of popular parallel filesystems (e.g., WAN-GPFS, Lustre-WAN). This will allow users to access files in a common filespace from different XSEDE resources hosted at different SP sites. The XWFS will particularly benefit science gateways (e.g. NanoHub, GridChem discussed above), since they need to manage task and data flows to and from many SP systems. Earthquake and cosmology data analysis exemplify applications that depend on multiple SP systems being able to "see" the same dataset.

As called for in the XD solicitation (p. 6), the GFFS consists of a global name space (i.e., a single, unified Unix-like directory structure), POSIX-like files, and XSEDE-aware filesystem drivers (e.g., FUSE [6]) that map the global name space into the local filesystem as a mount point. Applications and shell scripts can then access the resources in the GFFS as if they were local files and directories, eliminating the need to rewrite and customize applications to access remote XSEDE resources. The GFFS extends the usual wide-area filesystem paradigm in two ways: the types of resources accessible and the geographic and administrative locations of the resources. The set of resource types that can be accessed and manipulated within the XSEDE GFFS includes not just files and directories, but also services and other data types that can be made to *behave* like files and directories (e.g., instruments and relational databases), simplifying operations and reducing the learning curve for users. The GFFS extends the reach of XSEDE beyond the SPs into campuses, research labs, and other standards-compliant national CIs.

Among our examples, plant science, brain science, and epidemiology will be major beneficiaries of the GFFS, as will the widely cooperative projects in particle physics and earthquake engineering. Interoperability with other CIs such as OSG and DEISA will also benefit. By encompassing hierarchical filesystems, this approach will enable a coordinated archival approach to assure persistence of important datasets beyond the lifetime of particular service providers. As we have seen, this is crucial for Grand Challenge projects in particle physics, cosmology, and plasma physics.

Campus Bridging. As computational methods become increasingly central to the everyday scientific enterprise, the need to access large-scale compute and data resources and interact with distant colleagues becomes more acute. This is recognized by the NSF *Dear Colleague Letter: Cyberinfrastructure Framework for 21st Century Science and Engineering* (CF21) [7], by the inclusion of a task force on Campus Bridging within the NSF Advisory Committee for Cyberinfrastructure (ACCI), and more concretely within the XD solicitation (p. 8).

The XSEDE team embraces the NSF vision for a national CI. XSEDE may be extended out beyond the SPs to include user- and community-defined resources including:

(1) data resources (e.g., files, directory trees, relational databases, instrument and sensor data streams and repositories, and community collections).
(2) compute resources (e.g., clusters, clouds, servers, application gateways, desktops, queues, brokers, and virtual machine images).
(3) security resources (e.g., credential and authorization services for access control and Secure Token Services for group management).
(4) learning and workforce development among CIOs, VPs for research, researchers, faculty, students, and IT staff (as described in PD3.4 TEOS Plan).

These may be personal machines or resources located on campuses or within research labs or government, industrial, and academic settings (see PD3.2 XSEDE Architecture, §D.4.3 Campus Resources and PD3.2 XSEDE Architecture, §E.2.5 Federation Examples). These remote, peer resources will use the same tools, services, and interfaces used to access and operate XSEDE SP resources.

Our examples in storm prediction, brain science, and particle physics, as well as science gateways, critically depend on the campus bridging capabilities.

Improved Communication. As distributed computational workflows and pipelines consisting of pre-process, process, post-process, visualize, data staging, and so forth become prevalent, it is essential for clear, timely, and consistent information to be provided to users and workflow engines to report status and behavior of applications, dataflows, and services. The need for vastly improved communication to users about status, expected completion times, errors, diagnosis, and suggested corrective actions has been articulated again and again by users.

XSEDE has built-in notification services based on a standard publish/subscribe mechanism. Clients can request notifications (extensible to email or SMS) when jobs begin, complete, terminate, or otherwise change state. Job information is logically centralized, and logs showing the various actions performed on the job, resources consumed by the job, *stderr* files from a running job, etc. are made readily available to users and service provider personnel alike.

Standards-Based Implementation. The XSEDE team is committed to building its grid infrastructure based on applicable and broadly supported standards. Numerous user-expressed complaints regarding currently supported TeraGrid middleware focus on its limited interoperability with other infrastructures and the considerable variability between supported releases in the functions and interfaces provided. Users currently have few choices in terms of client tools and interfaces beyond the cumbersome command-line “reference implementation” tools provided by the middleware developers. In contrast, XSYS services will be capable of interoperating with any standards-compliant components. This has been demonstrated in XSEDE using UNICORE 6 [8] services deployed with production TeraGrid resources interacting with Genesis II [9,10] clients. Additionally, interoperability has been successfully demonstrated with our DEISA/UNICORE partners and our UK NGS colleagues (who use GridSAM [11], a third, independent standards-compliant middleware stack).

Integrated Design. The XSEDE architecture is conceived holistically, both with respect to itself and in regard to other systems. There are a small number of driving principles and concepts (PD3.2 XSEDE Architecture, §C.1.1 Design Themes) defining a small number of powerful primitives, which are combined and re-used in many different ways. Every “thing” is a resource with an identity, an interface, metadata, and possibly state. Similarly, all resources are accessed the same way, whether they are large resources like *Kraken* or *Ranger* or small desktop PCs. Security (including identity federation) is built into the basic communication fabric from the beginning.

The current toolkit-based grid middleware components supported in TeraGrid provide application programmers considerable flexibility but at the often prohibitive cost of investing themselves in a deep understanding of the complex (and often changing) low-level primitives and proprietary interfaces provided. The XSEDE team will relieve researchers of this burden, because researchers typically lack the relevant expertise and cannot afford to invest the resources to develop and maintain it over time. Indeed, developers understandably prefer to focus their efforts on science application development, and XSEDE’s design seeks to maximize their productivity by providing standards-based interfaces rather than toolkit-specific methods. In this way, XSEDE’s design also promotes the expansion of computational research to new and currently underserved scientists and disciplines.

Focus on Quality. Providing and sustaining a reliable system is essential to XSEDE’s success. Therefore, the XSEDE architecture includes in its foundations the mechanisms to support a wide variety of fault-detection, notification, and recovery services, together with flexible quality-of-service controls for different resource types and applications (see PD3.2 XSEDE Architecture, §E Quality Attributes). Quality attributes were considered early in the design process: fault detection, notification, and recovery mechanisms are built in, as are mechanisms to support replication for performance and availability. Usability, which drives adoption more than any other factor, has also been a focus since the project’s inception, as has the need for extensibility to support future needs both anticipated and unknown.

To ensure that the architecture reflects both current and future needs, the XSEDE team has adopted a stakeholder-driven architecture development process (see PD4.5 Systems Engineering Management Plan). We have generated our requirements from detailed stakeholder input; using a spiral process, additional requirements are continually generated and assigned to a subsequent development increment. Once requirements are generated, the design and development process begins its next iteration. During development, standard software engineering practices such as code reviews, test case development, unit tests, user panels, and regression testing will be performed. Before deployment, integration testing and extensive pre-deployment testing will be performed (see also PD4.5 System Engineering Management Plan, §E.4 Testing).

Smooth Inclusion of Cloud Resources. Cloud computing is widely perceived as a useful evolutionary step in large-scale enterprise computing (mostly due to cost efficiencies) and with potential in the computational science communities. Commercial availability of cloud services, primarily on large systems optimally designed for other purposes, have potential to provide useful burst strength for capacity computing loads where the usual lack of excellent inter-node communication is acceptable. The XSEDE architecture can readily extend into the cloud to exploit cloud resources for capacity computing as needed using the same mechanism used for campus bridging.

D.4.1.2 XSEDESystem Overview

We have chosen for XSEDE's grid infrastructure, XSEDESystem (XSYS), a Service Oriented Architecture approach with web services as the fundamental interaction paradigm [12-25]. We will employ selected standard specifications and profiles as the starting point for the fundamental basic services including grid-based execution, directory services, and flat-file and relational data management. We will closely track OGF, OASIS, IETF, and other applicable standards bodies to identify the conventions that will best serve the needs of the XSEDE stakeholders. We expect the XSEDE applications to be able to access resources (particularly data resources) overseas and vice versa via standard interfaces, enhancing collaboration opportunities for both communities. Thus, the XSEDE architecture implementation is striving for an artful mixture of standards where appropriate and compliant best-of-breed implementations of those standards.

XSEDE is a three-layer distributed systems architecture consisting of an access layer, a services layer, and a resources layer. The **access layer** provides a means for users to interact with the grid, whether it is via a custom application, a web portal or gateway, a set of APIs, or the GFFS. The access layer is where we meet our simplicity and ease-of-use objectives and provide a stable platform for users and application developers (see PD3.2 XSEDE Architecture, §D.2 XSEDE Access Mechanism). The **services layer** provides a standard set of interfaces upon which implementers of the access layer can depend. This is where execution, data, naming, directory, discovery, security, federation, and fault-tolerance service interfaces (called porttypes in web services) and protocols are defined. We will be using standards from both the web services and grid communities. Indeed, our initial configuration consists of interoperable components from two different middleware stacks, UNICORE 6 and Genesis II (see PD3.2 XSEDE Architecture, §F Deploying XSEDE). Finally, the **resources or provisioning layer** provides the physical or virtual resources that are being manipulated, whether they are computing systems, flat files, relational databases, or virtual organizations. Different vendors or implementers may provide different implementations of the grid services that map to their particular resources. It is important to note that the resource base may include service providers as well as campus, department, and individual resources such as local filesystems containing instrument data. Further, we have gone to great lengths to minimize what is required for a resource provider in terms of intrusiveness into their operational environment (see PD3.2 XSEDE Architecture, §D.4 Resources Layer)

D.4.1.3 XSEDE Architecture Implementation

The XSYS grid services are implemented with best-of-breed, standards-based components, specifically with UNICORE 6 as the backbone execution management middleware at the SPs. GPFS-WAN and Lustre-WAN constitute the XSEDE-Wide File System (XWFS), and the Global Federated File System (GFFS) is drawn from Genesis II.

UNICORE 6, led by a team at the Forschungszentrum Jülich (FZJ) in Germany, has been in production for over a decade. It is the grid software stack underpinning DEISA and is one of the three middleware stacks being distributed as part of the European Middleware Initiative. The UNICORE project has been a European leader in grid standardization and as a result implements many of the standards critical to our architecture. UNICORE 6 has a comprehensive set of user-facing tools to start and manage jobs, including workflows, across heterogeneous resources using standard mechanisms. By selecting UNICORE 6 for XSEDE, we ensure interoperation with European grid infrastructures, reduce costs, leverage an extensive existing software base, and reduce the risk of vendor lock-in by focusing on its standards-based aspects.

Genesis II is a standards-compliant grid middleware stack developed at the University of Virginia by a team that has been implementing large-scale distributed meta-systems since the early 1990s including Mentat, Legion, and Avaki [26,27,28,29,30,31,32,33]. Genesis II implements and integrates the standards and profiles emerging from the OGF Open Grid Services Architecture (OGSA) Working Group [34,35,36,37,38,39]. Genesis II has been used in production in the Cross Campus Grid (XCG) that spans the University of Virginia and Virginia Tech since February 2008. The XCG is used as both a compute and data grid providing secure transparent access to data in labs and on clusters. There has been an emphasis on ease-of-use, best exemplified by the Genesis II installer. The installer is designed to be "as easy to use as TurboTax," requiring no knowledge of grid protocols or web services.

The authentication and authorization mechanism in XSYS is built upon widely agreed upon web services and IETF and OASIS standards and specifications. In particular, we will be using RFC 5280 compliant certificates, WS-Trust, and WS-Federation for identity federation and signed SAML assertions compliant with InCommon Federation guidelines [40] ensuring the smoothest possible integration with campus IT infrastructures (see PD3.2 XSEDE Architecture, §D.1.3 Security and PD3.2 XSEDE Architecture, §E.2 Security & Federation).

Because of our standards-based strategy, other implementations besides UNICORE 6 and Genesis II may be used by campuses, or indeed XSEDE itself, in the future. For example, GridSAM[5], implemented and used in the UK could be used for compute management or Gfarm (Japan) [41] or iRODS [42] for implementation of file and directory services. This is a significant implementation advantage as it simultaneously reduces vendor lock-in and the risk of having any given project fail and increases the resources that can be accessed via XSEDE.

D.4.1.4 Preliminary Results

An interoperable, standards-based implementation has never been used in a production grid environment. All past grid infrastructures have been "monocultures" that use a single software stack. To address the risk of a new approach as well as ensure that the requirements and use cases can be satisfied with our planned implementation, we have performed three development increments (see PD6.11 Architecture Supplement: Development Increments). These increments were designed to validate our standards-based, artful mixture approach and to uncover problems and gaps that would prevent full production operation.

During the course of the development increments, we successively extended and tested XSEDE functional capabilities and quality of service attributes. The first increment, 0.1, focused on basic interoperability between UNICORE 6 and Genesis II, testing job-based interoperation. We followed that up in increment 0.2 by deploying UNICORE 6 and the GFFS at the centers, and the full Genesis II stack (GFFS and compute) at the University of Virginia and Virginia Tech. We then ran a series of functional tests against requirements and use cases, including executing a workflow, reading/writing GFFS from/to different sites, and meta-scheduling across campuses and centers. Increment 0.3 focused on quality of service tests, such as GFFS performance and availability, and the transition strategy for science gateways by porting a component of the RENCI Biomedicine and BioPortal Science Gateway.

We have successfully used these design increments to reduce risk, build the team, and validate our architectural approach. We have clearly demonstrated that we can meet the requirements and satisfy our use cases. We have learned places in the implementation that will need early attention, such as security interoperability, RNS integration with UNICORE 6, and timely and informative notification of job failure. We have built consensus around the architecture and plan and cultivated an *esprit de corps*, both internally and with our UNICORE 6 partners.

D.4.1.5 Architecture Team

The Architecture Team will consist of the Chief Architect, Deputy Architect, representatives from each of the four partner SPs, a part-time project manager, a documentation and training materials developer, and several software engineers. Most of the software engineers have several years experience in large-scale distributed systems (including fault-tolerance and availability techniques, performance optimization, security, distributed filesystems, and scheduling), testing, packaging, HCI, standards, and modern software engineering practices. The personnel will be distributed between the partner SPs, the University of Virginia, and FZJ.

D.4.2 XSEDE Operations

XSEDE Operations will provide ongoing centralized, production-level services to all users of XSEDE. Specifically, XSEDE Operations is tasked with deploying, tuning, and maintaining:

1. 24x7 frontline user support, deployment, monitoring, and management of all servers for all centralized production resources through the 24x7 XSEDE Operations Center.
2. Automatic distributed accounting and account management.
3. Deployment, testing, and maintenance of XSEDE capabilities and services in the production XSEDE environment.
4. Data management and coordination including XSEDE-wide parallel filesystems, data movement and management, and distributed archival replication.
5. Networking implementation and support and facilitating end-to-end performance for users.
6. Cybersecurity including a shared certificate authority and two-factor authentication system spanning all XD Service Providers (SP) and integration with campuses.

Below, we discuss these several functions in detail.

D.4.2.1 Operational Functions

D.4.2.1.1 XSEDE Operations Center

The XSEDE Operations Center (XOC) is a 24x7 service and support center. It provides an initial point of contact for users, as well as the deployment, management, and monitoring of all production resources. The XOC will follow well-developed policies and procedures to achieve the highest level of XSEDE resource availability and the quickest route to technical solution for the users.

The XOC answers a toll-free number and email 24x7. All user contacts with the XOC will result in a ticket. If the XOC cannot resolve the issue immediately and it is not urgent, it is referred to the User Support Consulting Service at the appropriate site. If it the issue is urgent, the XOC will contact the on-call representative at the appropriate site. All user issues will be tracked by a full-featured enterprise-wide trouble ticket system. We intend to provide a response within 24 hours for every ticket submitted and will strive to close 80% of the tickets within two business days.

The XOC will also deploy, monitor, and manage all centralized production resources such as the XUP, the accounting database, and the XSEDE Certificate Authority. It will also monitor the production resources at the SPs. We will use state-of-the-art high availability and configuration control techniques to achieve and maintain a high level of quality assurance.

A monitoring system will be implemented to continuously monitor and verify XSEDE systems, networks, software, and services to ensure that XSEDE provides the highest possible quality of service to users and stakeholders. The 24x7 helpdesk will follow established procedures in the case of unplanned outages to notify users and on-call personnel at local centers.

D.4.2.1.2 Accounting and Account Management

The Accounting and Account Management (AAM) team will provide continuity to the NSF HPC user community during the transition from TeraGrid to XSEDE. We plan to continue the support of the TeraGrid-developed AAM data repository and protocols. We have found them to be an effective solution for the storage and tracking of AAM data within a complex grid environment, and all of the SPs have already created production interfaces to this database. In addition, Blue Waters has chosen to use this database for its AAM needs.

This team will develop improvements such as a web interface to search for job-level data from XSEDE resources, support real-time query capability for end-users of allocation usage monitoring, support real-time access for ad hoc queries, develop a single-source resource description repository, and streamline the account request process. All of these improvements were based on user requirements as shown in PD3.5 Input Report. A centralized AAM system will build upon the TeraGrid development efforts to streamline request processing. Timely creation of approved accounts is an important metric for user satisfaction, and XSEDE will strive to complete the process for all users within five business days while maintaining a stringent security review of new user account requests.

D.4.2.1.3 Software Support

The Software Support team will deploy, test, and maintain the collection of software needed to implement the XSEDE cyberinfrastructure. This team will also coordinate the efforts to deploy the software at the XSEDE Service Provider sites including deploying testbeds or reference implementation for acceptance testing of the software before production deployment. The acceptance testing is an important part of our quality assurance efforts and will make use of the readiness criteria developed as described in PD1.4 Project Execution Plan, §E.4.1 Assuring Quality and Establishing Operational Readiness Criteria. This software includes data management and movement, coordinated scheduling and job submission, and science gateway portals as described in the XSEDE Architecture (§D.4.1).

D.4.2.1.4 Data Management and Coordination

The Data Management and Coordination team will support coordinated data services such as XSEDE-wide parallel filesystems, data movement and management, and a framework for distributed archival replication. Access to a global XSEDE-wide filesystem has been one of the top user requirements in every TeraGrid user survey, and we intend to meet that need with XSEDE. The XSEDE design described in the architecture document (see PD3.2 XSEDE Architecture) countenances several classes of filesystems that, together, will serve this spectrum of requirements including a wide-area, inter-SP filesystem. It is important that the global filesystem eventually supports multiple, distributed metadata servers and presents a sense of data locality allowing both performance enhancement and a soft-decay capability in order to support local access to local data even with degradation or loss of wide-area network links. Wide-area filesystems have not yet completely matured among filesystem software vendors, consequently, we view it to be prudent to pursue least two approaches within XSEDE. The XSEDE members have extensive experience with both Lustre and GPFS as implemented in a wide-area environment, and we plan to support both in the early years of XSEDE. There is already a wide-area Lustre effort within TeraGrid, and this will be continued. Further, IBM has provided XSEDE with attractive licensing terms for the use of GPFS across XSEDE (PD4.4 PEP Supplement: Project Planning, Management, and Execution, §D.1.3.4 Technology Providers).

The Data Management and Coordination team will explore and deploy a framework for a distributed archival replication service in consultation with NSF. In moving to a sustainable archival storage model for XD, it is essential that a community of SPs assume responsibility for long-term data storage, both for long-term data availability and to survive localized data loss. We propose to designate two types of data on long-term storage media: data that has been migrated locally from disk as part of normal hierarchical storage management and data that the users have designated for long-term archiving. The first is primarily the responsibility of the local service provider, except for distributed replication of this type of data, while the second must be cared for by the XSEDE organization as a whole. Quotas and usage policies for the SP-specific data are determined by the SP. Any XSEDE-archived storage approaches, e.g., replication and retention beyond the life of the originating SP, may require allocation. The XSEDE management will propose that an appropriate long-term storage allocations process is instituted and will attempt to provide funding by 1) encouraging researchers to write the costs of long-term storage into their proposals, and 2) working with the NSF to provide additional funding allowing XSEDE to more fully provide general long-term archival services for the scientific community. To encourage this, XSEDE will provide two replication servers to enable SPs to connect their archives to a collective replication service; these servers will be located at two separate sites to provide for high availability, and they will provide a catalog of replicated data and metadata. The servers will run data grid software to support simplified management of replicated objects and will also provide additional data transfer mechanisms for access from desktop systems without special client software. SPs will not be required to provide additional replicated storage capabilities but may choose to link their archives and other storage systems into the XSEDE-managed replication grid, providing centralized access and replication mechanisms to the XSEDE user community. The replication servers will also host a small amount of cache storage to facilitate transfers of large amounts of data to and from tape archive systems at high speed.

In addition, existing archival systems present multiple interface styles (e.g. “read-write” and “get-put”), recognizing the performance differences between disk and tape. As is discussed in PD3.2 XSEDE Architecture, the architecture provides for standard, generalized services for copying data between storage systems with diverse interfaces. XSEDE will propose to SPs a “standard” interface offering for these operations. The normal XSEDE prioritization mechanisms are being used to determine the scope of our initial efforts on this front.

D.4.2.1.5 Networking

We have identified a number of networking capabilities needed at the start of the project: addressing bandwidth size and stream duration, network load distribution, and data retention and storage. After assessing several options, we have developed a plan to deploy a network (XSEDEnet) that will be both extensible and responsive to changing requirements and technical capabilities. Initially, XSEDEnet will retain the current TeraGrid networking equipment at Starlight in Chicago to accommodate current TeraGrid RPs as well as current and future XSEDE SPs. We expect each SP to be connected to the Chicago hub by at least a 10Gb/s connection and have a second 10Gb/s connection to one or more of the national Research and Education (R&E) networks such as National LamdaRail or Internet2. After the first year, expansion will continue by extending the star topology by negotiating a Service Level Agreement with an R&E network to peer with XSEDEnet at the Chicago hub with at least 10 Gb/s connectivity. In addition, Blue Waters has indicated that they plan to connect to XSEDEnet in Chicago.

XSEDEnet will be specifically designed to adapt to the changing composition of the XSEDE environment in response to the addition of new SPs, new user communities, and new applications. In addition to providing a production infrastructure, the networking effort will include network services and support as well as expert consulting to deal with end-to-end network performance and data movement issues for both SPs and campuses. XSEDEnet will have the flexibility to tailor specific services to the needs of individual projects, even if the services are not yet network standards. We will also explore deploying state-of-the-art technology for exploiting dynamic bandwidth between SP sites and user sites on XSEDEnet. To better evaluate networking conditions, a monitoring infrastructure, consisting of both monitoring platforms and evaluation mechanisms, will be deployed in order to evaluate, maintain, and evolve XSEDE network services over time. We will use this information in deciding how and with which organization to extend XSEDEnet into peering with an R&E network.

XSEDE networking services will provide consulting to users and their campus network engineers to optimize end-to-end network performance that is important to applications requiring network communications across a distributed environment. Support will be available to aid remote users in improving end-to-end access, both to debug existing installations and topologies and to help design new ones.

D.4.2.1.6 Cybersecurity

The Cybersecurity team will deploy a centralized certificate authority for XSEDE. This will allow XSEDE to grant grid certificates at the same time as user accounts, and it will make it easier for users to use the XSEDE architecture. In addition, two factor authentication schemes will be deployed for greater protection against credential theft. Authentication will be implemented in a way that enables campuses to integrate with XSEDE through InCommon by taking advantage of the CILogon service [43]. The Cybersecurity team will also coordinate incident response across sites as well as perform security audits for SP sites to maintain the highest level of security in our interconnected environment. Please see PD5.4 PEP Supplement: Operations Planning, §C XSEDE Cybersecurity Plan for a detailed plan.

D.4.3 XSEDE User Services

XSEDE will support thousands of people who use its high-end resources directly to develop applications, submit jobs, and analyze and store data and many thousands more who use data collections, portals, and science gateways. XSEDE's user community will be very large and diverse, for four primary reasons:

1. broad science and engineering mission of NSF, spanning most fields of science and engineering.
2. diverse advanced digital resource types funded by NSF OCI as part of XD.
3. federation with other high-end CI centers and to bridge to campus CI infrastructure.
4. support of users with computational expertise varying from beginner to expert.

The XSEDE architecture, systems engineering approach, management plan, and policy structure were designed to work together to enhance the productivity of every user in this diverse community, while making XSEDE even more reliable, capable, secure, and easier to use than the current TeraGrid. However, it is XSEDE User Services that will provide the foundational *support* for this community as part of an integrated spectrum of support services. This support is part of an integrated spectrum—comprehensive in both technology coverage and user expertise—and will be offered through a variety of interfaces, methods, and formats. XSEDE will work with the XD Service Providers (SPs) to offer the services that support this community. The primary focus areas for User Services are: 1) Online Information, 2) Allocations, 3) User Engagement, and 4) Training. These support activities will leverage the extensive experience of XSEDE staff. These activities are summarized below; more details are provided in PD5.3 XSEDE Operations Plan, §D User Services.

D.4.3.1 Online Information Resources

Providing online information is the most effective means of continuously supporting thousands of remote users. The web, laptops, and mobile devices have become fixtures in our daily lives, and users are no different: their expectations of what can be accomplished online are set by their daily use of such technologies in other aspects of their lives. It is therefore crucial that XSEDE provide high-quality, comprehensive content through these familiar but increasingly powerful interfaces.

XSEDE User Documentation and News: The NSF-funded high-end computing centers have provided web-based documentation for many years, but there are still many improvements that can be made to the current TeraGrid user documentation. XSEDE will make several key improvements, including:

- ***Integrated, complete* set of user information**: This includes new/beginning user documentation, user guides for every digital resource, and instructions on how to use XSEDE resources and services in workflow applications, for maximum throughput, etc.
- ***Consistent* user guides**: Currently, TG RPs create their own system user guides, but XSEDE will work collaboratively with SPs to develop user guide templates for each resource type (HPC, visualization, storage, etc.), with as much consistency as possible in the sections spanning these resource types.
- **User input on documents**: Users will be able to provide comments and feedback directly on documents. User Engagement activities (see below) will collect additional information through monitoring user forums and asking specific questions in user surveys and focus groups.
- **Better revision information**: Every document will show its date of last modification and include a link to a chronological list of revisions enabling easy review of changes since last reading.

XSEDE will continue to provide User News online through the web ('pull') and via subscriptions to receive items by email ('push') and as RSS feeds (hybrid). Improvements over TG User News will include making all user-relevant events (training classes, allocations teleconferences, allocations deadlines, etc.) available via standards-based calendar feeds and providing the capability to receive reminders of deadlines and of user events receivable via SMS alerts.

XSEDE User Portal: TeraGrid User Portal (TGUP) has been an outstanding success. The majority of TG users now use it regularly, not only to find information but to apply for and manage allocations, to monitor systems, to move files and data, and even to access TG systems through GSI-SSH. Building on the success of the TGUP, the XSEDE User Portal (XUP) will present ever more user-centric information and enable users to access TG services interactively and easily. XSEDE staff (who are the developers of TGUP) will offer increased functionality in the XUP with a huge array of features within the first month of operations by porting them from the TGUP, including:

- Request, manage allocations
- Reading user news, documents
- Requesting technical support
- Participating in user forums
- Comparing, monitoring systems
- Managing files and data
- Accessing systems
- Reporting problems and issues
- Signing up for TEOS events
- Editing profile information
- Noting publications, grants
- Using remote visualization

The initial feature set will include everything above in addition to what is already in TGUP. The XUP team will add customization capabilities to enable users to personalize XUP to make it most effective for their computational research/education. After adding customization and completing the interactive feature set including job submission and workflows, the XUP will even be able to serve as a rapid prototyping environment for future science gateways.

Mobile Devices: Virtually every researcher now has a smartphone, and these devices are rapidly increasing in capability. The TGUP already has a mobile interface; XSEDE will create a much more capable one for XUP. XUP-Mobile will be organized to leverage the strengths of smartphones—alerts and status updates, news, short documents, touch-based actions—while still providing access to the full range of XUP through a web interface. Feedback through the XUP-Mobile itself and from user surveys, focus groups, and tickets will be used to add and modify features.

Social Media: Social media services such as Twitter and Facebook have achieved tremendous penetration and are now used by businesses and organizations to reach customers, supporters, etc. Social media have an important role in XSEDE TEOS activities (§D.6) to enhance the learning process by connecting users to each other and to experts. Facebook could help users contact each other and share experiences and results, forming a virtual community; Twitter could serve as a means of providing alerts and updates. The XSEDE User Service team will evaluate the opportunities presented by social media tools and include them in XSEDE's online information as they prove effective.

D.4.3.2 Allocations

The XSEDE allocation process will build and improve upon previous TeraGrid efforts to provide the simplest, most flexible, and most equitable allocations procedures. Three main objectives help define XSEDE allocations procedures:

1. minimize the barriers faced in applying for resources.
2. provide users with access quickly whenever possible.
3. maintain an appropriate level of review for scarce, valuable resources.

The process in XSEDE will be similar to the current NSF/TRAC process. PIs will submit requests, the requests will be evaluated, and allocations will be awarded. XSEDE improvements will handle the increased diversity of XD digital services, simplify the submission process, and minimize the time to access.

Broaden Allocation Types: The NSF high-end computing program has historically allocated only HPC resources, while providing 'unlimited' archival storage. The relatively recent addition in TG of visualization and high-throughput computing (HTC) resources and the increasing demands on storage resources have necessitated some modifications to extend allocations to these resource types. However, even these resource types will require substantial improvements in XSEDE allocations procedures:

- **Storage:** already being allocated in TG, but XSEDE will distinguish different levels of storage in performance (flash vs. disk vs. tape), duration of usage (short term vs. allocation-length vs. very long term), community vs. group/individual use, etc.
- **Visualization:** again, we are already doing this in TG with XD Visualization, but XSEDE will distinguish interactive usage from batch, explore prioritization of interactive usage, and consider including an option to allocate real-time visualization consulting for interactive usage.
- **Throughput:** XSEDE is learning from OSG on this and hopes to include OSG as a full SP for providing this capacity. XSEDE allocations will also be extended to resource types that enable high-throughput and on-demand computing as they are proven effective at scale for open science and are integrated into XD (e.g. computing clouds).
- **Advanced Support for Research Teams (ASRT):** This program, described §D.5.1, builds on the TG ASTA program to provide research teams with collaborators from XSEDE staff for a specific application enhancement project up to one year in length.

We expect to further broaden resource types to account for experimental systems and grids, data collections with access limitations/privileges, use of federated CI centers and campus CI resources, etc. XSEDE will broaden the process in each phase—application/request, review, and management—to account for an increasing diversity of high-end digital service types. More information about this can be found in PD5.3 XSEDE Operations Plan, §D.2 Allocations.

Requesting Allocations: XSEDE will simplify the request interface, building on recent TG efforts but further reducing the complexity and the time between request and granting of allocations for the majority of our users. A front-end interface to the proposal process, designed to efficiently guide users through the proposal process, will be featured in the XUP. XSEDE will simplify allocation requests by introducing Standard Allocations in addition to Startup Allocations. Standard allocations are significant but fixed amounts of resource or service allocation, specified for each resource or service. This will accomplish two main objectives: 1) removing the need for most XSEDE users to specify in laborious detail their allocation needs and 2) enabling review within the XSEDE team, speeding the time to approval to a maximum of two weeks while easing the burden on the peer-review allocations committee. Standard allocations allow XSEDE to make rapid assessments of projects through a "Does the work fit under the standard allocation?" criterion rather than detailed computational justifications. A short form concept will be used to greatly simplify the requests for these standard allocations. Obtaining supplemental resources within a user's current allocations period will require the long-form XRAC process so that proper justification can be given.

Startup allocations will be further enhanced to support users new to XSEDE. Currently, these awards are reviewed internally, are relatively easy to obtain, and have resource availability as the primary review criterion. We will add the option of requesting easy to access personal support from the XSEDE frontline user support. We will also provide interactive support capability for users submitting proposals (i.e. a phone hotline or internet chat capability). Finally, we will explore the viability of providing essentially *immediate* access for new users to *one* XSEDE system so that users can quickly start experimenting with the full XSYS stack and XSEDE user environment, start testing codes, etc. This has significant security considerations that will be fully explored between XSEDE and the SPs once the architecture implementation has begun.

Additional allocation types will be based on user requirements and will be flexible throughout the life of the XSEDE project. A beginning set of these will include Education, Development, and Research allocations. The Development type will allow users to request interactive open-ended access to resources for debugging and benchmarking (on those resources that allow such usage); the Research type will be reserved for production computations. Education allocations are for workshops and courses. Science gateways (SG) will be serviced by Community allocations where the justification will be based on serving a particular scientific community. These types will assist both reviewers and users in how best to express what they need of XSEDE. We will add additional types as necessary in response to user needs.

Reviewing Allocation Requests: Peer-review is a key component to equitable, merit-based access to the resources provided by NSF. XRAC will incorporate evolutionary changes to the current TRAC process and will focus on a more streamlined and efficient process while continuing the necessary stewardship of expensive, unique, and finite resources. All large requests (above the new Standard Allocation limit for a resource) will be reviewed quarterly by the XRAC. A set of external reviewers, comprised of academic professionals with computational domain expertise, will be recruited to form the XRAC.

A network of internal reviewers, made up of members of the XSEDE staff (we expect to have approximately 20-30 persons from scientific support staff, including at least one from each XSEDE Service Provider), will be available for review on a rolling basis for non-XRAC requests—startup and standard—so that reviews happen shortly after submission of a completed request.

Thus, there will be three levels of allocations: small (Startup, Education, Development, and Research), standard, and XRAC (including Supplemental). The first two levels will be performed completely by internal review on a rolling basis, which will ensure getting users to computing quicker. Small requests will require at least one internal reviewer to quickly assess the request and grant it based on availability within one week. Standard allocations will be evaluated by up to three internal reviewers for reasonableness of scientific approach, resource appropriateness, and scientific funding. It will involve coming to a consensus review in no longer than 14 days. XRAC reviews are for any request for more than the standard allocation specified by the Service Provider or for Supplemental requests for additional computing. They will be handled at a quarterly review panel meeting of external reviewers, similar to the panel meetings held in the current TRAC process. XSEDE staff will still prescreen all requests to the XRAC for compliance and completeness and will provide feedback to proposers if there is any missing or insufficient justification. XSEDE staff will also ensure that all requests that result in reduced or zero allocations are provided with clear explanations of reasons and suggestions for what to include the next time, what kind of allocation to request, etc.

XSEDE Allocations Management: Again, the XUP will be based on the current TGUP to provide a means for users to easily monitor usage and manage allocations across all XSEDE services. This functionality will continue to be improved, including easy delegation of allocations managers for projects and the ability to create user accounts and place per-user allocations limits for allocations. We will also enable the PI and the designated allocations manager to request automatic monthly usage reports and will provide automatic notifications when allocations levels have dropped below 10%, when allocations deadlines are within two weeks, and other alerts as deemed valuable through the User Engagement feedback processes. We will also add a command-line interface for accomplishing this on each system (though this CLI will be local to the system and not span systems, unlike the XUP interface).

D.4.3.3 User Engagement

User Engagement is a set of XSEDE activities that will provide direct assistance and inputs for all other areas of XSEDE: from other user services to architecture (features, capabilities, usability, etc.) to operations (environments, policies, etc.) to advanced user support. User Engagement activities include both reactive support and proactive discussion and solicitation of feedback and requirements.

Consulting: Addressing user requests for assistance rapidly and accurately is important for ensuring that users are productive *and* satisfied. Even the best documentation can sometimes require a substantial learning effort to answer a question that professional staff can answer in minutes. Therefore, XSEDE will continue to provide a two-tiered consulting solution for XSEDE users: frontline helpdesk for rapid responses as part of the operations activities and routing of more advanced questions to the appropriate XD SP or XSEDE staff, as required.

The current TG consulting process works well, leveraging custom consulting software developed by XSEDE staff at NCSA and an interface developed by TGUP staff at TACC. XSEDE will improve the coverage of the software for the diverse resource types of XSEDE. XSEDE will also improve the ability of the software to enable users to identify distributed problems and for XSEDE operations staff to mark tickets as such and to direct them to multiple relevant parties with notes describing why solutions require joint/coordinated responses. The revised consulting system will also enable staff to tag tickets as possible reasons to update user documents, add to FAQs, etc.

A Consulting Coordinator will oversee the execution of the overall process from submission to solution to improvement of other services. The Consulting Coordinator will monitor accuracy and quality of responses, verify that tickets are being routed to the most effective responders, measure time-to-solution, ensure that tickets involving multiple services are being handled effectively, and coordinate with other parts of XSEDE to help improve services based on user tickets.

User Feedback Collection: User Engagement activities will include a much greater amount of *proactive* gathering of user feedback than in the current TeraGrid. Proactive support will include:

- Mining (automated and human) support tickets, including tagging tickets that can help improve XSEDE with redirection to appropriate XSEDE leaders/managers.
- Active participation in online user forums (in the XUP).
- Annual user surveys, prepared and analyzed with external, professional help.
- User focus groups quarterly to solicit inputs not easily garnered from surveys.
- “Shoulder surfing” with new users to observe how they use the web site, XUP, systems, etc.

Each of these activities provides complementary information that will be used to improve XSEDE services. The User Engagement manager will oversee the execution of the feedback collection activities by XSEDE and XD SP staff and will route inputs to the appropriate staff for consideration.

Interface with Technology Insertion Service: The XSEDE team won the XD Technology Insertion Service (TIS) award. XSEDE User Engagement will interface with XSEDE TIS activities in two ways: through the TIS Usage, Satisfaction, and Impact measurement activities and by providing user feedback regarding TIS selection of technologies to evaluate. XSEDE’s executing the TIS award means that XSEDE User Engagement staff can easily provide inputs—collected through the means described above—that help the XSEDE TIS team make XSEDE more usable and capable, as well as more robust and secure.

D.4.3.4 Training

The current TeraGrid offers a loosely coupled portfolio of training activities that are essentially RP workshops offered on RP calendars, with a few more coordinated efforts among them and a common calendar on the TeraGrid web site. XSEDE will present a much more unified training program in design as well as appearance to users. In addition, Training is linked to Education and Outreach activities by the XD solicitation and logically due the spectrum of the audiences and purposes for each. The User Services training activities are therefore discussed in §D.6 (Training, Education, and Outreach Service), but it will be fully integrated into the User Services program as well via the online information resources.

D.4.3.5 User Services Transition to XSEDE from the TeraGrid

While implementing the XSEDE architecture will require time and significant effort, the transition of user services will be almost transparent. The TGUP is developed and supported by the same XSEDE staff that will develop XUP. The TG allocations process is also already coordinated by XSEDE staff and uses software (TGUP, POPS) developed by the XSEDE institutions. The XSEDE User Engagement activities will be staffed by personnel from NCSA, NICS, PSC, and TACC, who already support the majority of TeraGrid projects and users on their current systems. The helpdesk is manned by XSEDE staff, who already handle most of the consulting tickets—again, using software developed by XSEDE staff. Most TG training is offered in support of the users of systems at XSEDE sites. In short, the XSEDE partners operate the largest TG systems, support most TG users, develop and support most TG user services-relevant software, and offer the most TG training already. The XSEDE plans will improve these user services activities, but there is essentially no risk and minimal effort in this transition.

D.4.4 XSEDE Project Office

D.4.4.1 Governance, Collaboration, and Federation

The XSEDE project is managed by the University of Illinois (Illinois/NCSA) with key partnerships (via sub-awards) to University of Tennessee at Knoxville (UTK/NICS), University of Texas at Austin (UT Austin/TACC), MPC Corporation/Carnegie Mellon University/University of Pittsburgh (PSC), University of Virginia (UVa), and other partners who strongly complement their expertise. Illinois is responsible for: satisfactory project execution, sub-award management and oversight, subcontracts, procurements, and timely submission of reports as requested by NSF. The project team consists of highly qualified senior staff members with extensive and current experience executing large projects, high-performance computing operations, and distributed environments.

The XSEDE project will be managed through a tightly integrated, distributed organization with clearly defined roles and responsibilities at each level. The governance model is geared towards inclusion of, and responsiveness to, users as well as XSEDE partners and NSF. While there is great strength in the diversity of sites and services, they will be brought together into a single integrated whole with this plan. A critical aspect to the management structure is that, following project management principles, there will be very clear control points—individuals in the organization with responsibility for specific project scope, schedule and costs—and decision authorities matching the WBS (work breakdown structure), so that decisions can be made efficiently by each level of the organization.

Organizational vision will be determined by the XSEDE senior management team (described below), which includes the chairpersons from the User Advisory Committee and the XD Service Provider Forum (see below) to ensure direct stakeholder input. This vision will be communicated and executed via meetings and reports (PD5.1 Communications Plan). Although the organization chart is hierarchical, there will be lateral communication among organizational elements, e.g. cross-cutting discussions among systems engineering, architecture, and operations groups. Figure 1 shows the organization chart, including the relationship with advisory committees.

XSEDE Senior Management Team: The XSEDE senior management team consists of: the PI/Project Director (Towns); the directors of XSEDE Operations (Andrews), Users Services (Boisseau), Advanced User Support (Roskies), and Education and Outreach (Lathrop); the Senior Project Manager (Boudwin), the Senior Systems Engineer (Brown), the Chief Architect (Grimshaw), the Chair of the User Advisory Committee (TBD), and the Chair of the XD Service Providers Forum (TBD). The senior management team will meet on a bi-weekly basis to assess project status, plans, and issues. This team is constituted from those responsible for the day-to-day operation of the project and is the highest level management body in the organization. In order to be responsive to both the user community and the set of Service Providers with whom we will collaborate, the chairs of the User Advisory Committee and the XD Service Providers Forum are members of this team.

Although the XSEDE partners have extensive reach for qualified staff within their institutions, we recognize and have identified qualified individuals outside our team—specifically with the competing XROADS team—with whom we plan to expand XSEDE's expertise.

Internal and External Oversight: XSEDE is a complex project and needs both internal and external advisory mechanisms to ensure: a) timeliness and technical quality in design and implementation, b) relevance and usability of the resources and services provided to the community, and c) effective synergy with the other CI initiatives within the nation and around the world. Functional relationships among project components, advisory groups, and the community at large are depicted in Figure 1. In order to remain well informed of the requirements of the user community, XSEDE leadership will receive advice and counsel from the User Advisory Committee (UAC), the XD Service Providers Forum, and the Strategic Advisory Board. These advisory committees will be intimately involved with XSEDE management in guiding the project towards optimal operations, service, and support for users.

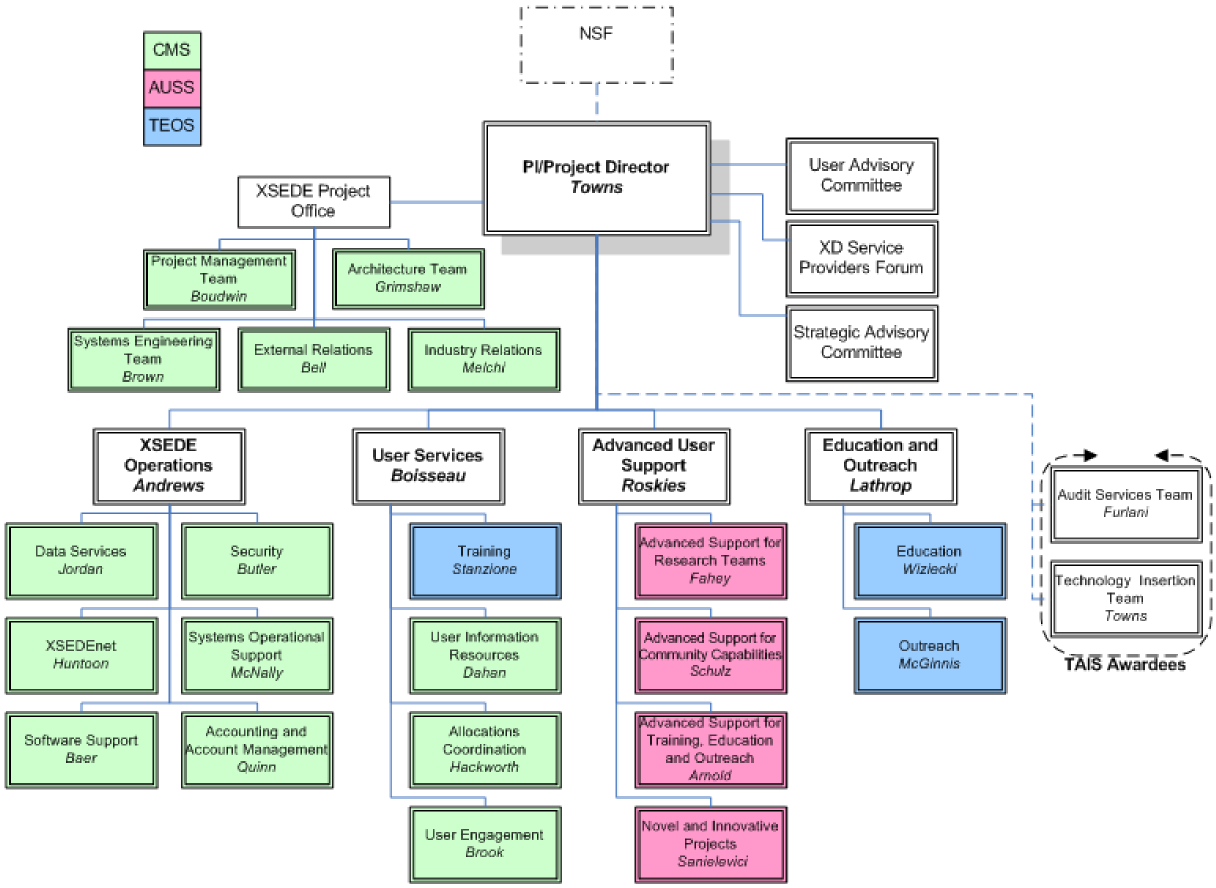

Figure 1: XSEDE Project Organization Chart

- The **User Advisory Committee** will comprise members of the national community who represent the needs and requirements of the research and education community and will provide guidance with respect to how the activities and plans of XSEDE can better serve those needs. UAC members will be selected by the XSEDE senior management team from the user and prospective user communities with input from NSF directorates to include broad range of representation across disciplines. The approximately 20 members will select the committee’s chair who is an XSEDE senior management team member. The committee will formally meet quarterly and represent the “user’s voice” to XSEDE management.
- The **XD Service Providers Forum** will consist of representatives from all XD Service Providers and other XD program awardees. Members will select a chair who is an XSEDE senior management team member. They will exclude from consideration representatives from the XSEDE proposing institutions. The forum is the means by which all Service Providers have input into XSEDE’s management and will present issues, recommendations, and feedback on proposed changes to the XSEDE environment and services.
- The **Strategic Advisory Board** will include highly respected leaders from academia, industry, national laboratories, and other federal agencies. Membership input will be solicited from the user community, NSF, and leadership of other CI projects such as OSG, LIGO, LHC, DEISA, NAREGI, and others. The committee members will select a chair and meet semi-annually as a high-level board to advise XSEDE senior management on vision and planning.

Special advisory subcommittees may be convened to address specific topics as they arise. Each will be headed by an advisory committee member and may include members outside of the established advisory committees. A subcommittee of the Strategic Advisory Board on Training, Education, and Outreach has already been established.

Organizational Quality: The management and governance structures are designed to align with the interrelated Core Values and Concepts of the Baldrige National Quality Program [44], which are: visionary leadership, customer-driven excellence, organizational and personal learning, valuing workforce members and partners, agility, focus on the future, managing for innovation, management by fact, societal responsibility, focus on results and creating value, and systems perspective. Included in the annual report (PD1.4 Project Execution Plan, §F.8 Reporting) will be a self-evaluation of the project based on the Baldrige National Quality Program criteria.

Work Breakdown Structure and Project Deliverables: The project has been organized around project deliverables grouping the project's discrete work elements (or tasks) into a work breakdown structure (WBS) to organize and define the total project work scope. The WBS, WBS dictionary, and assignment of responsibilities are provided in PD1.4 Project Execution Plan, §G Work Breakdown Structure. The management structure has been created so that each scope of work is assigned to a specific level 3 WBS manager, who is then accountable to the WBS level 2 directors who are on the XSEDE senior management team. Each WBS level will be assigned scope, schedule, and budget responsibilities with the decision making and control described in PD1.4 Project Execution Plan, §K.1 Change Control Process. The project has also developed a systems engineering process (§D.4.4.3) for continuous improvement and inclusion of new and evolving requirements with a specific methodology for promptly gathering, reviewing, approving, and assigning responsibility for incorporation and execution of new requirements through standardized project processes.

External Coordination: While XSEDE is a well-defined virtual organization, there is an extended set of partners with whom XSEDE will have various relationships. The extended organization created by the amalgamation of XSEDE and other separately funded bodies will be referred to as the XSEDE Federation. The relationship between XSEDE and various partners will range from intimate (TAIS Technology Insertion Service (TIS)) to definite (XD Service Providers, TAIS Technology Audit Service (TAS), CI providers, vendors) to peripheral (some entities in other countries). All formal relationships will be documented via agreements that must cover a wide spectrum in both the services and responsibilities involved. Many of these agreements will be specific to the particular partner, but we categorize them into a small number of groups, based on the type of partner. These agreements will form the underpinnings of a pervasive cyberinfrastructure ecosystem.

The types of agreements anticipated by XSEDE are described in more detail in PD4.4 PEP Supplement: Project Planning, Management and Execution, §D Management of Formal Relationships.

Industrial Program: The four industrial programs engaged in this proposal–NCSA’s Private Sector Program; PSC’s Corporate Affiliates Program; TACC’s Science & Technology Affiliates for Research Program; and the NICS Industrial Partnerships Program–bring industry to the table to use the centers’ advanced resources and services to drive scientific achievement, increase national competitiveness, and improve the economy. More than one-third of the Fortune 50 companies have worked with us. This team of centers is superbly qualified to promote and share the benefits of the XSEDE digital technologies and services with industry. The XSEDE partnership will engage American industry by leveraging the powerful industrial programs that exist at the service providers to provide additional knowledge sharing, research, technology transfer, and training opportunities to the industrial user community. In addition, XSEDE has an industry representative on its strategic advisory board.

Leveraging extensive training classes and additional tailored training activities, the XSEDE industry program will help industry to address its primary challenge in using advanced digital resources: the shortage of trained talent. Industry partners will be asked to provide input on workforce requirements so that training classes may be further tailored to their needs. Additional efforts will be focused on training courses that specifically address the needs of small and medium enterprises (SMEs). Reports from the Council on Competitiveness indicate that SMEs are not advancing in the use of modeling and simulation.

The XSEDE service providers will use their current industrial partnership programs as a springboard to reach these firms by coordinating marketing and outreach materials and programs.

In addition, XSEDE will run an open competition for industry to propose an innovative software development project that could either be a completely new code written from scratch or modifying, rewriting, or porting an existing application. The intent is for the application to run at scale on multiple XSEDE resources. XSEDE and the industry partner will commit staffing resources to support the final project that is selected. The new software must be publicly available.

D.4.4.2 Project Management

The project management (PM) team members have extensive experience applying project management principles to large, complex, distributed projects including projects in the private sector, government, and TeraGrid. The experiences of the team members and best practices will be combined to provide professional project management that is critical to the success of XSEDE.

The PM team developed and will maintain a *Project Execution Plan* (PD1.4 Project Execution Plan), which establishes the means to execute, monitor, and administer XSEDE. The PM team will select and adapt appropriate project management practices and tools going forward to accommodate evolving XSEDE project needs and provide the discipline of planning, organizing, and managing resources to bring about the successful completion of project goals and objectives. The PM team will also provide communication and integrated reporting to all project stakeholders—NSF, the XSEDE partner institutions, the Service Providers, and the users. It will also manage the baseline change control process. The PEP will include all elements delineated in the NSF solicitation for full proposals and describe the execution processes for management of the project, establish project baselines against which the project will be measured, and serve as the primary reference document for the project.

Baseline Change Management and Risk Management: Each year the project will determine the schedule, budget, and scope to be accomplished, and this information will be documented in work packages at level 3 of the WBS, providing the project baseline from which to measure project accomplishments. Changes to these baselines (cost, schedule, and scope) will be managed through a change management process with change thresholds described in the PEP. If a change request is significantly complex, the Project Director (PD) may convene a Change Control Board (CCB). The CCB will consist of the PD, the level 2 WBS managers, the chief architect, and the lead systems engineer. Others may be asked to contribute their expertise depending on the nature of the change request.

Risk management is incorporated into the project at all WBS levels. The NCSA risk tool—originally developed for the Blue Waters project—is used for risk identification and monitoring, and the PM team provides expertise and guidance to WBS managers so they can effectively manage risk for their work scope. As risks are added, changed, or retired, they will be captured and updated regularly in a published risk register. The risk management process is described in the PEP and PD5.4 PEP Supplement: Project Planning, Management and Execution, §C XSEDE Project Risk Management Plan. An initial risk assessment has been executed with high risk items and mitigation strategies included in the PEP and all identified risks recorded in PD4.6 Risk Register.

Schedule and Milestones: The PM team, in conjunction with the WBS level 3 managers, has developed a series of near-term and out-year activities organized into work packages necessary to complete the XSEDE goals and deliverables. The duration and interconnectivity of these activities is captured in a schedule baseline subject to the change control process and measureable milestones developed for tracking and reporting progress. The PM team and WBS level 3 mangers will continue to evolve out year planning packages to work packages each year, allowing for continuous inclusion of new requirements and recommendations. The detailed schedule is available in PD4.1 Resource Loaded Project Schedule.

Project Reporting and Communications: The project will provide NSF with regular updates via teleconference, as well as formal quarterly and annual reports including information from the Service Providers as well as progress against the PEP to provide an integrated view. Communication is key to the success of any endeavor and especially for a large distributed project. PD5.2 Communication Plan links all project groups and describes communication methods and frequencies. The Communication Plan will maximize the effectiveness and efficiency of project communications, providing information in the right format, at the right time, and with the right impact.

Management of Transition from TeraGrid: XSEDE is committed to a seamless transition from current TeraGrid operations to the start of XSEDE. A key requirement in all of our planning has been to assure there is no interruption in services at the hand-off from TeraGrid to XSEDE and throughout the XSEDE project period. TeraGrid to XSEDE transition activities will be coordinated by the PM team. All members of the XSEDE PM team are also current members of the TeraGrid Project Management team; they will be responsible for tracking transition activities, resolving issues, and reporting back to XSEDE management. Tim Cockerill, the current TeraGrid Area Director for Project Management, will serve as the overall coordinator of transition activities.

D.4.4.3 Systems Engineering

XSEDE is committed to enhancing productivity for its users and other stakeholders by providing an environment that demonstrates excellence and a continuously improving experience. In addition, it will be responsive and adaptive to evolving demands and resources throughout the performance period. Satisfying this commitment requires greater attention to detailed engineering activities than was necessary in the formative days of grid supercomputing. System engineering provides a disciplined and repeatable approach to integrating diverse activities so they are complementary and efficient. It is a strategy for managing complexity and smoothly evolving the system in response to shifting technology, science goals, and user communities. The XSEDE approach to systems engineering marks the transition of the TeraGrid to a new level of maturity in its engineering practices. The approach builds on best engineering practices, but adapts them to meet the unique technical, institutional, and social challenges of XSEDE, while maintaining XSEDE's user focus.

The overall engineering process is documented in PD4.5 XSEDE Systems Engineering Management Plan (SEMP). It covers topics such as: planning, requirements analysis, functional analysis, system analysis and control, sustainment, testing, and integration. XSEDE Systems Engineering is responsible for defining, evolving, and executing the SEMP. The key elements of the engineering approach are 1) combined spiral system development with agile software development; 2) emphasis on the user in all aspects of engineering; and 3) adoption of a rigorous architecture-centric approach to achieving sustainable improvements in system quality. These are briefly described in the following sections.

Spiral Systems Engineering and Agile Software Engineering: XSEDE combines a *spiral* systems engineering approach for systematic and planned evolution with an *agile* software engineering approach for integrating the complex and individually evolving components of XSEDE. Spiral system development permits a graduated and risk-mediated approach to development. Each spiral increment delivers new quality or functional capabilities, phased in a way that exposes technical risks early while still providing flexibility to adapt to changing technology and user needs. The SEMP documents seven spiral increments—four development increments (three completed during the XSEDE planning process) and three deployment increments (PD4.5 SEMP §E.5.4 Identified Increments). Additional development and deployment increments are anticipated.

Agile software development (see PD3.1 Requirements, §D.4.1 Agility vis-à-vis XSEDE) is required to meet the challenge posed by the reliance of XSEDE on a substantial number of off-the-shelf components and technologies, almost all of which are evolving at different tempos, and to meet the needs of many different user communities. Agile integration permits the acquisition of "just in time" expertise in fast changing technologies, permitting risk-reduction experiments for requirements analysis and architectural design (see PD6.11 Architecture Supplement: Development Increments).

Emphasizing the User in All Engineering Phases: A key feature of XSEDE is its emphasis on the user in all engineering phases, as summarized in Figure 2. User Engagement (§D.4.3.3) identifies new requirements as a result of continuous contact with XSEDE users through consulting and feedback mechanisms such as focus groups and ticket mining. The user requirements evaluation and prioritization (UREP) working group is responsible for formalizing and approving new requirements. Usability panels are established for each *deployment* increment (nominally scheduled at six month intervals) to assess the operational readiness of new releases, as well as to provide feedback to XSEDE architecture and engineering. (See PD4.5 SEMP, §E.1.6.2 Requirements Validation)

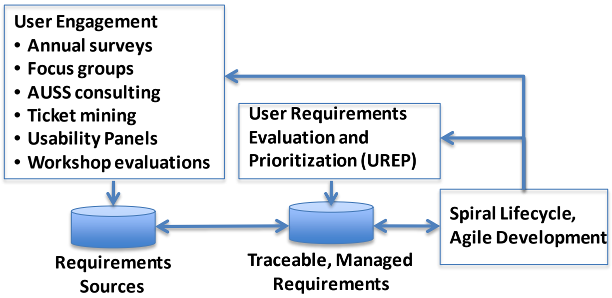

Figure 2: User-Centric Requirements

Commitment to Sustained Quality Improvement: The XSEDE architecture (§D.4.1) provides flexibility and extensibility to address emerging user needs and new technologies; XSEDE Systems Engineering provides the disciplined engineering processes to ensure that flexibility and extensibility does not come at the expense of system quality. The systems engineering team uses metrics to assess adequacy and sustainability of all engineering processes, from the capture of potential requirements through requirements validation, implementation, testing, deployment, and sustainment (PD4.5 SEMP, §D.5.8.5 Process Reviews).

XSEDE will employ a repertoire of proven processes, methods, and techniques to deliver predictably high quality technologies and services to its users. One paradigmatic method that simultaneously engages users (and other stakeholders) and exposes critical system quality attributes is the Architecture Tradeoff Analysis Method (ATAM) [45], developed by the Software Engineering Institute at Carnegie Mellon University and extensively used for over ten years in systems engineering projects at all scales. ATAM uses *quality attribute scenarios*, defined by stakeholders, to identify critical system quality requirements. It also makes the connections between science drivers and quality attributes explicit and identifies architectural risks in satisfying these requirements. Ultimately, quality attributes are reduced to technical performance measures (TPMs). For example, job failure rate (0.5%); job failure notification rate (5 minutes); and others (PD4.5 SEMP, §D.5.7.1 Identification of Technical Performance Measures). ATAM and its variants (quality attribute and mission thread workshops) have been tailored and used throughout the XSEDE planning phase (PD3.1 Requirements, §D.3.2 Architectural Approaches to Quality Attribute Analysis). For example, ATAM has been applied to the XSEDE architecture and XSEDE services. Because ATAM is also a key gateway between major steps of the spiral process, it will continue to be used as XSEDE progresses and as new stakeholder needs surface.

Figure 3: ATAM Method

D.4.4.4 External Relations

A centralized, professional External Relations (ER) team will directly contribute to and broadly disseminate XSEDE's long-term success and the success of its users. The XSEDE External Relations team will be responsible for communications that promote high-end digital services, their scientific value, and their social impact to the science and engineering community, to NSF and other agencies, and to the public. These communications will highlight the enabling role the resources, technical expertise, innovations, and services provided by the XSEDE staff and collaborating organizations play in each case. Outcomes of research and education conducted using XSEDE resources and services will frequently be used as the touchstone for describing the impact of NSF's investments. The ER team will be an integral part of the XSEDE management and reside organizationally in the XSEDE Project Office, giving the team the clearest possible understanding of the leadership's goals, plans, and immediate needs.

The team will be able to proactively disseminate messages and successes as they happen and broadly distribute integrated multimedia marketing materials with consistent messages among numerous media outlets. XSEDE ER efforts will expand on TeraGrid's efforts along several dimensions, including leveraging social media, actively engaging users to identify story ideas, and expanding media relation efforts. Communications within this integrated marketing approach will include print materials and annual flagship publications that highlight science and engineering breakthroughs and training, education, and outreach successes. The ER team will also be responsible for the overall information architecture of a comprehensive public website, which will include introductory and explanatory information about the overall XSEDE project and news and video content. Social media is a growing part of any marketing strategy, and the XSEDE ER team will work to broadcast XSEDE's message through a variety of social media outlets (initially Twitter, Facebook, and LinkedIn). A proactive application of social media will allow the project to identify new topics of interest and concern and to interact directly with interested audiences on these topics, especially younger members. The ER team will work closely with XSEDE's TEOS efforts to ensure that training, education, and outreach are well publicized. The two teams will also collaborate on establishing, promoting, and supporting a set of online communities, including traditional and social media-based discussion forums.

D.5 Advanced User Support Service

The XSEDE Advanced User Support Service (AUSS) will bring the best available knowledge and skills to bear on the most challenging science issues to maximize the impact of science and engineering results achieved by the XD user community. XSEDE's senior personnel established the Phase II TeraGrid's advanced user support program in 2005, and roughly ¾ of the experts currently working in this program are from XSEDE's lead institutions. *Many users we interviewed to gather requirements for XD identified* ***human expertise*** *and* ***support people*** *as* ***the best thing about the Phase II TeraGrid.*** Accordingly, we will leverage this expertise already in the team as the foundation of XSEDE AUSS and will recruit additional expertise from staff at other SP sites (including those participating in XROADS) and from external experts from the community. This will allow us to broaden the span of our capabilities to provide excellent and capable advanced user support, while assuring a smooth transition from TeraGrid. Our plan conforms to Advanced User Support suggestions made by the TeraGrid's Scientific Advisory Board [46].

A central lesson learned by XSEDE partners in our decades of providing leading edge advanced resources to the national research community is that *effectively using multiple technologies to facilitate scientific progress requires a cadre of talented staff professionals*. These professionals possess combined expertise in several fields of computational science and engineering. They have a deep knowledge of underlying computer systems and of the design and implementation principles, tips, and tricks for optimally mapping scientific problems, codes, and middleware to these resources. AUSS will include experts in not just the traditional use of petascale computing systems but also in extreme digital data management, workflow engineering, and the creation and maintenance of scientific gateways.

There will be several thrusts that go beyond the advanced support in the current TeraGrid. One is that XSEDE AUSS will focus on *novel user communities and innovative applications*. Fully 25% of AUSS efforts will specifically seek out and address these novel challenges. We will aggressively develop projects in new science areas that have traditionally not participated in HPC and collaborations with researchers and educators from underrepresented groups, e.g., at minority-serving institutions (MSIs) and EPSCoR institutions.

Another major innovation of XSEDE is *flexible funding within AUSS*. There will be areas of expertise that users will need that will not be present on our staff, whether in domain knowledge or in computational application development and tool productivity. We will cultivate and leverage ties with other centers of expertise (DoE Office of Science labs, NNSA labs, DOD centers) and supplement our expertise by using an open process to engage consultants from the academic community.

Two other major advances beyond current TeraGrid activities will be an increased emphasis on the optimization of currently or potentially widely used community codes, with a focus on helping projects funded by NSF programs (e.g. PetaApps, SDCI, STCI, SI^2, MREFC) to generate optimized, robust, sustainable, maintainable community applications; and the professionalization of the management associated with AUSS projects (see PD3.3 AUSS Plan).

In XSEDE, advanced user support projects will complement the operational helpdesk and user engagement work that is coordinated under CMS. As a rule, an AUSS project will require no less than 1 FTE month. The AUSS director, deputy director, and team leaders (see §D.5.5 below) will work with the CMS User Engagement team to proactively identify areas and user groups that need advanced support. We will take into account the advice of the User Advisory Committee and the need to broaden access in terms of fields of science, institutions served, and demographics. We will aggressively solicit candidate science or engineering research problems that require or can exploit petascale computing capabilities, seek collaboration with funded projects such as PetaApps, and coordinate with the NSF science directorates. We will also support training, education, and outreach programs in TEOS to foster integration of research and education and will provide AUSS resources for facilitating community portals via science gateways. Needs for advanced support will also be identified by the User Services Allocations team, for which all AUSS members will serve as internal reviewers. The XSEDE Operations Center will identify common user problems based on reports from the ticket system that indicate the need for advanced support, and other referrals will be generated by TEOS activities. Leads from all these sources will be referred to the AUSS management team, which will contact the stakeholder in question and lay the groundwork for the establishment of well-defined and realistic work metrics and deliverables.

AUSS projects fall into four categories, which are further described below. They are Advanced Support for Research Teams (ASRT), Advanced Support for Community Capabilities (ASCC), Advanced Support for Training, Education, and Outreach (ASTEO), and the Novel and Innovative Projects (NIP) that can intersect with any of these.

D.5.1 Advanced Support of Research Teams

An *Advanced Support of Research Teams (ASRT)* project is a collaborative effort between an XSEDE user group and one or more AUSS staff members, the goal of which is to enhance the research group's capability to transform knowledge using XD resources and related technologies. Typical ASRT projects will last for six months to one year and might include the optimization and scaling of application codes to use 10,000–way parallelism or more per job; aggregating petabyte databases from distributed heterogeneous sources and mining them interactively; or helping to discover and adapt the best work and dataflow solution for simulation projects that generate ~100 TB of persistent data per 24-hour run. The XSEDE ASRT program will build upon the TeraGrid ASTA program and will complete any ASTA projects that are active at the start of XSEDE.

A request for ASRT support will be made by the principal investigator of the research team via the resource allocation process. If the request is recommended by the reviewers, and if staff resources are available, a statement of work for up to one year will be developed by the PI, the ASRT leader, and the AUSS project manager. It will include a staff assignment from the pool of available advanced support experts who have the necessary skills. The project plan will be approved by the AUSS deputy director. The ASRT leader, working with the AUSS project manager, will be responsible for project tracking and reporting and for requesting additional resources or assistance from XSEDE management as needed.

D.5.2 Advanced Support of Community Capabilities

Advanced Support of Community Capabilities (ASCC) efforts are aimed at deploying, hardening, and optimizing software systems necessary for extensive research communities to create new knowledge using XD resources and related technologies. ASCC projects will include collaboration with the developers of widely used community codes and tools and may include industrial partners. Projects of this type will also support communities that wish to use XD resources via science gateways and/or data repositories.

ASCC projects will be proposed to the AUSS director by the ASCC leader based on input from AUSS, CMS, TEOS, and TIS user engagement teams. Each proposal will outline how the work will benefit a well-defined and extensive user community and why it is expected to have significant scientific impact. Priority will be given to helping projects funded by NSF programs (e.g. PetaApps, SDCI, STCI, SI^2, MREFC) to generate robust, sustainable, maintainable community applications. The proposal will outline the timeline, deliverables, and the ASCC staff requirements, as well as a sustainability plan showing how the resulting software will be made available to the target community and maintained after the ASCC project ends. In evaluating ASCC proposals, the AUSS director will consult the User Advisory Committee and then decide which ones we should support. For each approved ASCC project, the ASCC leader will work with the code developer and the AUSS project manager to develop a full statement of work and sustainability plan. The ASCC leader working with the AUSS project manager will be responsible for project tracking and reporting and for requesting additional resources or assistance as needed.

D.5.3 Advanced EOT Support

Many activities organized by XSEDE TEOS will require technical content to be developed and presented by AUSS experts. AUSS work in support of TEOS (*ASTEO*) will include the development and delivery (in person and/or online) of training modules on petascale programming techniques, both general and specific to each XSEDE system; modules on workflow building, using co-scheduled data transfers, data reduction concurrent with simulation, and algorithms for petascale data mining; and participation in scientific conferences to present the results of relevant advanced user support projects. ASTEO staff will be on the front lines of engagement with current and prospective users and will refer information and leads to AUSS management for follow-up action.

The ASTEO leader will work with the TEOS management team to develop specific training, education, and outreach activities that require technical content to be developed and presented by AUSS experts. For each such activity that entails more than travel (tutorial, workshop, mentoring, lecture, etc.), the ASTEO leader and the AUSS project manager will produce a statement of work. The project plan and the staff assignment must be approved by the AUSS director. The ASTEO leader, working with the AUSS project manager, will be responsible for project tracking and reporting and for requesting additional resources or assistance as needed.

D.5.4 Novel and Innovative Projects

Novel and Innovative Projects will be specifically targeted at advanced support for **broadening participation in XD.** The NIP leader and staff will work closely with the XSEDE outreach team to seek out user groups, communities, and digital services that have not benefitted from traditional HPC approaches but that now stand to benefit from the quantitative and qualitative revolution brought about by XSEDE. Examples of *novel science areas* might include biodiversity, linguistics, and social networks. Examples of *demographic diversity* will include researchers based at MSIs and EPSCoR institutions, SBIR recipients, etc. Examples of *innovative technologies* might include applications supporting mobile computing clients and seamless integration of distributed, heterogeneous databases. Suggestions will be sought from advisory bodies, NSF program directors, and XSEDE internal resources, including TEOS and TIS.

AUSS staff members with expertise in related disciplines and technologies, and with a talent for technical outreach and needs-analysis, will be dedicated to pursuing such projects and developing them into ASRT or ASCC work plans. These staff members may then be assigned as part of the team that executes the resulting projects. Specifically, we anticipate that many novel and innovative projects will entail the development and operation of ***science gateways, data repositories, and campus bridging solutions***.

D.5.5 AUSS Management

Co-PI Ralph Roskies will direct overall AUSS activity, manage the process for identifying and filling needed expertise, interact with the User Advisory Committee, and supervise the AUSS line management team. This team will comprise the AUSS deputy director and the leaders for ASRT, ASCC, ASTEO, and NIP. The CMS PM team will provide one of its members to serve as AUSS project manager, ensuring that all AUSS projects and processes are managed according to the XSEDE-wide practices. This management team will be responsible for the selection and execution of all AUSS projects. They will assign staff teams to projects by mapping available skills to needs, and they will manage the AUSS resource planning process. See PD3.3 AUSS Plan for the detailed description.

D.6 Training, Education, and Outreach Service

The TEOS mission is to recruit, prepare, and support a large and diverse scientific academic and industrial workforce capable of advancing scientific discovery through the application of computational science and engineering, using the XSEDE cyberinfrastructure ecosystem. Numerous national reports identify the critical need for a larger and more diverse workforce able to utilize computational science and engineering (CS&E) to advance the nation's competitiveness and ability to innovate (PD3.4 TEOS Plan, §C.1). During the planning grant, TEOS user requirements were collected through interviews, focus groups, and discussions with 48 people from 29 organizations (PD6.3 TEOS Requirements Interviews Report). The figure below illustrates the breadth of TEOS services to be provided, as a direct response to the user requirements, in collaboration with all of XSEDE including CMS and more than six AUSS FTEs. TEOS partners (PD2.2 Proposed Institutions and Companies) include NCSA, NICS, PSC, TACC, Cornell University Center for Advanced Computing, Krell Institute, Ohio Supercomputer Center, Shodor, Southeastern Universities Research Association (SURA), and the Illinois I-STEM Education Initiative.

Education and Outreach are directed by Shodor (Lathrop), with Education managed by NCSA (Wiziecki) and Outreach managed by PSC (McGinnis). Training is managed by TACC (Stanzione) within User Services that is directed by TACC (Boisseau). The user requirements and evaluation process will be managed by NICS (Ferguson). The TEOS management plan is described in PD3.4 TEOS Plan, §C.4 TEOS Management. TEOS will continue to solicit user requirements to improve TEOS services in response to community needs. A TEOS Advisory Group will provide ongoing advice for improving TEOS services. The figure below illustrates how these services will be integrated to provide both skilled and next generation users with the assistance they need to succeed. With funding from NCSA Blue Waters, Lathrop will spend 0.5 FTE as the Blue Waters Technical Program Manager for Education and Outreach and leverage this leadership position to facilitate training, education, and outreach coordination across XSEDE and Blue Waters.

TEOS, in collaboration with CMS and AUSS, will work with TeraGrid to ensure a smooth transition from TeraGrid to XSEDE. The TEOS services described below improve upon TeraGrid by expanding the scope and scale of learning and workforce development, by providing in-depth support to engage new and under-represented communities, and by coordinating XSEDE campus bridging efforts. Details on the TEOS services to address user requirements are included in the planning document (PD3.4 TEOS Plan, §C.2 TEOS Services to Meet User Requirements).

D.6.1 TEOS Training Service 1: Expand Scope of XSEDE Certified Training

User requirement: Provide a broad range of quality training across critical digital services topics.

TEOS action: TACC will lead the effort to identify training topics to be developed and delivered on an on-going basis. TEOS will provide a new set of guided training roadmaps with links to XSEDE-endorsed training materials available via the XSEDE User Portal (§D.6.10). XSEDE-endorsed training, a new feature of CI training quality control, will include exercises and sample codes in response to user requirements. At least 10 new topics, based upon user and staff needs, will be developed annually including content on new digital resources, tools, and techniques. XSEDE will also work with discipline-specific projects to tailor training to meet their needs (e.g. iPlant Collaborative [47]).

To avoid duplication of effort and to help fill gaps in the roadmaps, TEOS will coordinate development of new content with organizations developing related content including Campus Champions, NSF/OCI Track 2 awardees, XD Visualization awardees, the NCSA Blue Waters Track 1 award, the Department of Defense PETTT program, and the Oak Ridge National Laboratory Leadership Computing Facility training programs. Blue Waters will contribute documentation/training materials, assist in the outreach activities including the Campus Champions program, and provide training content to the XSEDE community. To ensure the quality and usefulness of training materials, TEOS will facilitate an expert review of materials using the verification, validation and accreditation (VV&A) process [48]. Formal VV&A reviewed materials will be tagged as XSEDE-endorsed materials and added to the roadmaps in the XSEDE User Portal. Informal reviews (Amazon-style) will be solicited from the user community.

D.6.2 TEOS Training Service 2: Expand the Scale of Training

User requirement: Provide training that minimizes travel and addresses just-in-time learning, makes training accessible from the desktop, and provides training on more campuses.

TEOS response: TACC will lead the effort by expanding TeraGrid's training efforts to provide researchers, educators, Campus Champions, staff, and students across the country with at least 50 live training sessions annually. XSEDE will deliver these synchronously via web 2.0-based technologies to reach users at their desktops. XSEDE will expand the on-line tutorials and courses, offered by NCSA's CI-Tutor and Cornell's Virtual Workshop, by developing at least 10 new topics per year. Training will be enhanced with assistance from experts and the community through the XSEDE Learning Environment (service 10). XSEDE will offer a new "Train-the-Trainers" program to prepare Campus Champions, the SURA team, and others in becoming XSEDE Certified Trainers. This will prepare SURA to integrate training into TEOS outreach (service 8) with minority-serving institutions nationally.

D.6.3 TEOS Education Service 3: Certification and Degree CS&E Programs

User requirement: Provide computational science and engineering competencies to guide the education of the next generation of science, technology, engineering, and mathematics (STEM) practitioners.

TEOS response: OSC will review the draft CS&E competencies developed by the Ralph Regula School of Computational Science [49] and publish a final set of CS&E competencies. OSC will also lead the effort to assist institutions that are ready to implement a model CS&E program but are limited by current faculty expertise and the level of faculty effort required to create all of the necessary supporting materials and learning modules. These certificate programs will prepare future researchers as well as pre-service K-12 teachers. This will have the dual impact of preparing the future STEM workforce and improving the quality and CS&E skills of classroom teachers and higher education faculty. XSEDE will work with at least three campuses to incorporate undergraduate certification programs in year 1 and expand over time to support 6 undergraduate and 3 graduate programs per year. XSEDE has initial commitments to work with four 4-year colleges and universities and two 2-year colleges.

D.6.4 TEOS Education Service 4: Curriculum Development

User requirement: Assist faculty in developing undergraduate and graduate curriculum materials.

TEOS response: Shodor will lead the effort to assist faculty in developing content and pedagogy aligned with the CS&E and digital services competencies to prepare students across all STEM fields by integrating new models of teaching parallelism using emerging digital services. To impact K-12 education, TEOS will collaborate with teacher preparation faculty, with initial commitments from 6 institutions. XSEDE will work with faculty to modify 75 existing modules and create 50 new curricular topics/modules over 5 years. Faculty will be encouraged to take advantage of the full array of XSEDE training offerings. TEOS will offer 10 curriculum development workshops for educators throughout the year at multiple campuses through synchronous delivery. Emphasis will be placed on delivering content to MSI and EPSCoR institutions to enhance the CS&E curriculum among under-represented institutions. Through a new partnership with Sigma Xi [50], XSEDE will launch a new effort to visit one campus per month for 2-3 days of deeper on-campus work with faculty incorporating XSEDE resources into their curricula.

D.6.5 TEOS Education Service 5: Student Engagement

User requirement: Prepare and sustain a larger and more diverse pool of undergraduate and graduate students to be future researchers and educators.

TEOS response: Krell extends their success with the Department of Energy Computational Science Graduate Fellowship [51] by leading the effort to immerse undergraduate and graduate students in a new comprehensive program of training, internships and fellowships, mentoring, and recognition**.** Students will be recruited nationally, with an emphasis on under-represented students. Students will gain real-world research and development experience through internships. TEOS will support 50% of the costs of up to 40 students per year; the remaining funding will come from XSEDE teams and research groups providing internships. Mentors, coaches, and internship opportunities will be drawn from XSEDE teams and from among XSEDE users. Students will gain recognition by publishing papers, presenting at conferences, and participating in competitions. The Campus Champions (service 7) will form a new Student Champions program from among these students. TEOS external evaluation will track the students beyond the term of their internship to study the long-term impact of motivating these students to pursue CS&E studies and careers.

D.6.6 TEOS Outreach Service 6: Campus Bridging

User requirement: Provide campus bridging for users to access XSEDE resources and assist campus-level technology and policy planning to balance the use of local, regional, and national resources.

TEOS response: NICS will lead the XSEDE effort to bring together XSEDE staff with campus administrators (CIOs and VPs for research), IT staff, Campus Champions, campus PIs, and users. TEOS will coordinate information exchanges, training, CI Days [52] events, and strategic planning to help campus leaders, researchers, and educators understand how to balance the utilization of campus and XSEDE resources. These interchanges will inform XSEDE on how to improve services with campuses for users. Technical and usability requirements for campus bridging will be addressed through XSEDE architectural design and implementation, improving interoperability among CI resources on campuses and the XSEDE architecture. This service will directly address community needs described in NSF's CF21 document [7].

D.6.7 TEOS Outreach Service 7: Campus Champions

User requirement: Maintain the success of the TeraGrid Campus Champions program [53]; strengthen support for Campus Champions; help Champions be more effective on their campuses; avoid the sense of isolation (geographic or institutional) among the Champions; make the best use of limited resources; and involve students.

TEOS response: TEOS will build on the successful TeraGrid Campus Champions program by having PSC lead the XSEDE effort to provide deeper collaborations with Champions to better support and represent the needs of campus staff and users in utilizing XSEDE for research and education. Champions will have the opportunity to become XSEDE Certified Trainers, and will be encouraged to contribute campus-developed content to the training roadmaps. Champion sites will receive preferential consideration to host training and education workshops. The XSEDE Learning Environment (XLE) will include Champion-driven capabilities to build a stronger sense of community with other Champions, XSEDE staff, and users. As a new initiative to address geographic and perceived institutional isolation, XSEDE will develop Regional Champions to support smaller and under-represented institutions that don't have a sufficient user base or staff resources to become Champions. Regional Champions will utilize the XLE to build an effective distributed community. Student Champions will be identified on campuses to engage many more students and their research teams. This will broaden the XSEDE user base and increase the long-term impact of XSEDE. XSEDE will continue to pair consultants from AUSS with Champions, ensuring that campuses have the training and support they need to be effective.

D.6.8 TEOS Outreach Service 8: Engaging Under-represented Communities

User requirement: Engage and sustain a larger and more diverse population of CS&E practitioners and provide deeper support of under-represented communities on their campuses.

TEOS response: SURA will lead the effort to increase the number of under-represented institutions and individuals making use of XSEDE services and the number of under-served institutions participating in the Campus Champions program. To create sustainable CS&E peer-support communities among under-represented groups, the XSEDE team will host a minimum of three regional, multi-institution community-building events per year and schedule in-person visits to 8 under-represented campuses per year. Through these events and visits, XSEDE will identify user requirements, facilitate engagement with the AUSS team, and promote use of XSEDE services. XSEDE will provide virtual office hours through the XLE (service 10) to support on-going interactions between these new users and XSEDE experts from AUSS and the XSEDE community of users. During the first year, at least 20 new research and education projects from under-represented communities will be using XSEDE systems and services. The under-represented community will then grow by at least 25% per year.

D.6.9 TEOS Outreach Service 9: Speaker's Bureau

User requirement: Provide awareness of the benefits of XSEDE to research and education.

TEOS response: PSC will coordinate presentations, workshops, and exhibits at a minimum of six national professional society conferences per year. Emphasis will be placed on conferences with the potential for recruiting new communities of users. TEOS will work with User Engagement, CMS, and AUSS to cover the events and will work with the External Relations team to provide promotional materials, flyers, posters, and related materials. XSEDE will collect contact information from at least 10 attendees per day, and AUSS will follow-up to engage at least 10% of those contacts as new XSEDE users. Material from the Speaker's Bureau outreach efforts will be made available through the XLE for "virtual site visits" and orientation material for asynchronous community engagement.

D.6.10 TEOS Crosscutting Service 10: XSEDE User Portal for Learning and Workforce Development

User requirement: Provide a persistent, current repository of high-quality training, education, and outreach materials.

TEOS response: TACC will lead the effort to provide a new centralized "one-stop-shop" for access to TEOS resources through the XSEDE User Portal (PD5.3 XSEDE Operations Plan, §D.1.2 User Portal)**.** The XSEDE User Portal (XUP) will integrate functionality to address needs of researchers and educators, including a new curated XSEDE Resource Repository, roadmaps for quality training, support for user accounts for training events, tutorial materials, APIs for federated searches and access to XUP capabilities, and a new XSEDE Learning Environment. The XSEDE TEOS Resource Repository will enable sharing of quality reviewed materials with National Science Digital Library (NSDL) collections of education and training modules designed to serve K-20 audiences. Tutorial content will be made available via NCSA's CI-Tutor system [54] (used by more than 47,000 people to date) and Cornell's Virtual Workshop [55] (in use to support TACC *Ranger* training). The tutorial content includes more than 30 digital services topics that will be available upon the start of XSEDE. The new XSEDE Learning Environment, led by NCSA, will provide a new online learning environment that fosters both formal and informal learning focused on the use of XSEDE's digital resources. Individuals will be able to organize and manage their own learning. XLE will broaden the impact of XSEDE's training and education program beyond what could be achieved using traditional methods alone as well as increase social capital to build a robust community to broaden the use and support of XSEDE services. XSEDE will provide an API to allow science gateway developers to integrate the XSEDE federated search into their pages (in much the same way as domain-specific Google searches can be embedded into websites within the look and feel context of that web site) to allow gateways to search the TEOS Resource Repository. A second API will allow easy integration of XLE forums to science gateway sites, allowing gateway users to access forums of like-minded users (without the need to duplicate this functionality in every gateway).

D.6.11 TEOS Crosscutting Service 11: Learning and Workforce Development Audit and Insertion

User requirement: Adopt best practices and lessons learned into services to best serve users, integrate research and education, and advance CS&E learning and workforce development.

TEOS response: NICS will lead the effort to conduct an ongoing process of assessing community needs and requirements. TEOS will identify proven, successful strategies from among at least five external projects each year that will be considered for incorporation to improve TEOS and XSEDE services. The objective is to understand community needs and requirements, so that the resources and services can be agile and improve to address evolving user needs. Campus Champions will provide feedback to alert XSEDE to campus needs and concerns. Community input will be sought through surveys, focus groups, interviews, and face-to-face discussions with the community, the TEOS Advisory Group, and the XSEDE

User Forum. The information will be shared with XSEDE management to ensure that issues receive timely attention.

D.6.12 TEOS Crosscutting External Evaluation of Learning and Workforce Development

TEOS will employ an external evaluation, led by the I-STEM at Illinois, designed to provide formative information to guide learning and workforce program improvement and a summative assessment of program effectiveness and impact. The evaluation will utilize an educative, value-engaged approach (EVEN [56]) that outlines mechanisms for effectively incorporating cutting edge scientific content, strong instructional pedagogy, and sensitivity to diversity and equity issues into STEM educational programming. The evaluation will address four key areas: implementation, effectiveness, impact, and institutionalization. The process will include longitudinal tracking of student participants to assess the impact of XSEDE on their educational and career paths. The following metrics will be evaluated to assess the short- and long-term impact of TEOS programs:

- Contributions to, and use of, TEOS resources and materials by the community.
- Levels of user satisfaction across all target groups (from surveys, focus groups, interviews).
- Active engagement of critical individuals and user groups including users, Champions, CIOs, etc.
- Reduction in the gaps in training and education materials required by users.
- Evidence of improved research and educational outcomes by users.
- Number of CS&E certificate and degree programs created, enrollment, retention, and matriculation figures, and institutional demands for the programs.
- Case studies of institutional impact and change.
- Number and breadth of curricular materials available and used by the community.
- Number and diversity of students pursuing advanced CS&E studies and CS&E and HPC careers.
- Number of under-represented individuals using XSEDE on a sustained basis.
- Numbers of research projects, publications, and external funding associated with participation.

In summary, TEOS, in concert with CMS and AUSS, will provide national-scale CI and services. TEOS will contribute to the preparation of a larger and more diverse academic and industrial workforce. TEOS will engage new and under-represented communities in using XSEDE on a sustained basis. TEOS will work with campuses to extend digital services knowledge and capacity to advance computational science and engineering research and education. TEOS will continue to gather user requirements and external evaluations of its services to further refine and improve training, education, and outreach services.

D.7 Coordination with Technology Insertion and Audit Services

Ensuring that XD provides tremendous capability with maximum productivity will require both technology evolution and effective monitoring of systems, utilization, and impact—continuously, through the entire life of the project. OCI competed these activities in a separate solicitation from this current CMS, AUSS, and TEOS opportunity. The XSEDE team competed for that XD Technology Audit & Insertion Service, having deep expertise in particular in technology R&D, evaluation, and deployment. The final award was split: the XSEDE team was chosen to execute the evaluation and recommendation activities (Technology Insertion Service), while a team led by U. Buffalo was selected to conduct the independent monitoring activities (Technology Audit Service).

The XSEDE team began its TIS activities in April 2010, even though the official award was delayed for administrative reasons to the beginning of July 2010. The XSEDE team has created a web site and a TIS team wiki, drafted a database schema for tracking current and new CI technologies, and begun efforts to define and execute the formal technology evaluation process. The XSEDE TIS team has begun mining TeraGrid data—user surveys, consulting tickets, etc.—to help develop priorities for technologies to evaluate, and will canvas the attendees of TG10 to solicit further input. By the 6-month mark, the XSEDE team will have an open implementation of the XD Technology Evaluation Database (XTED) with the capability to accept community inputs on technology projects. It will also have a formal process and infrastructure for evaluating new technologies for recommendation and insertion into XD—a full six months before XD begins operations. The team will continue collecting data and evaluating technologies so that whichever teams is awarded XD will have prioritized community inputs to assist in evolving XD's capabilities.

The XSEDE TIS team will work most effectively with the XSEDE team for two main reasons. First is that the TIS staff are in the same organizations as the XSEDE Architecture and Operations staff. Even in virtual organizations, the benefit of proximity and relationships are substantial. Second is that the XSEDE team already operates most of the systems and services that will transition into XSEDE (see next section). For both of these reasons, technology insertion—which is actually more recommendation and collaboration to install and support—will be most easy for the XSEDE team to execute program-wide. However, the XSEDE TIS team's effort will be of great value regardless of which team receives the CMS/AUSS/TEOS award.

Another advantage of the XSEDE team executing the XD TIS award is that it has enabled XSEDE to already start coordinating with the Audit Service team. The Audit Service must remain objective, but it will still require the collection of data from the XD infrastructure that is enabled by the XD awardees' software stack. The XSEDE TIS team is able to start planning *now*, and because it overlaps with the CMS team, this information will be more easily implemented in XD at the outset.

D.8 Closing

XSEDE proposes an ambitious plan to provide unprecedented new cyberinfrastructure capabilities and to stimulate a national cyberinfrastructure ecosystem, while making everything easier and more reliable—more *productive*—than any other cyberinfrastructure to date. This project can only be achieved by a team possessing tremendous talent and leadership. We thereby close this proposal by summarizing the unique qualifications of the XSEDE team and leaders.

D.8.1 XSEDE Team: Unmatched Experience and Expertise

Our team draws from four of the most successful advanced computing centers in the world: NCSA, NICS, PSC, and TACC. These centers comprise the majority of staff in the TeraGrid—including the TG Forum chair—and offer the vast majority of resources, while handling most of the training and support as well.

The four co-lead institutions have a long history of collaboration. These centers have built relationships and developed trust that make for a cohesive team, overcoming the divisiveness that often plagues large distributed organizations whose members must frequently compete with one another on other fronts. This group been complemented by carefully chosen leading individuals and institutions in CI research, development, EOT, project management, and systems engineering. The whole is significantly greater than

Table 1: XSEDE Leadership in XD Program Awards to Date.

XD award	Institution Lead	XSEDE Lead?
Track 2A - Ranger	TACC	Yes
Track 2B - Kraken	NICS	Yes
Track 2D - Keeneland	GaTech (NICS/ORNL)	Yes (project director, and housed at ORNL)
Track 2D – Future Grid	Indiana University	Co-PI (with several XSEDE partners)
XD Visualization – Longhorn	TACC	Yes
XD Visualization – Nautilus	NICS	Yes
XD Technology Insertion Service	NCSA	Yes, with all four XSEDE co-PIs
Ember	NCSA	Yes
OCI "Dear Colleague Letter" systems	In negotiations	3 to 5 expected

the sum of its parts. It has grown into a true team.

D.8.2 XSEDE Leadership

Even the most talented team and the best-designed plan cannot *guarantee* success in an unprecedented endeavor of this complexity. Experienced, effective leadership is needed to ensure that the collective talents of a distributed team are organized to execute complex plans—and to change the plans as needed based on user requirements, technology evolution, and scientific opportunities. The XSEDE team is led by four of the most experienced CI leaders in the world, all of whom lead and manage very large activities spanning operations, support, education, and R&D.

John Towns is Director of the Persistent Infrastructure Directorate at the National Center for Supercomputing Applications (NCSA) at the University of Illinois. He is the PI on the NCSA Resource Provider/HPCOPS award for the TeraGrid Project and serves as Chair of the TeraGrid Forum—the forum providing overall leadership for the TeraGrid Project. He has gained a broad view of the computational science needs and researchers through his key role in the policy development and implementation of the resource allocations processes of the TeraGrid and preceding NSF-funded resources. His background is in computational astrophysics making use of a variety of computational architectures with a focus on application performance analysis. At NCSA, he provides leadership and direction in the support of an array of computational science and engineering research projects making use of advanced computing resources. Towns plays significant roles in the deployment and operation of computational data and visualization resources and grid-related projects.

J. Towns: *Ember: a critical science and engineering enabling SMP resource*, OCI 10-12087, $3,2M, 3/10-2/12; *Planning for XSEDE: the eXtreme Science and Engineering Discovery Environment*, OCI 09-41686, $1,6M, 4/09-7/10; *TeraGrid Extension: Bridging to XD*, OCI 09-32251, $30,2M, 6/09-3/11; *Leadership Class Scientific and Engineering Computing: Breaking Through the Limits*, OCI 07-25070, $208M, 10/07-10/12; *NLANR/DAST*, OCI 01-29681, $2.5M, 7/02-6/06; *National Computational Science Alliance*, OCI 96-19019, $249.1M, 10/97-9/05; *The TeraGrid: Cyberinfrastructure for 21st Century Science and Engineering*, SCI 01-22296 and SCI 03-32116, $44.0M, 10/01-9/05; *Cyberinfrastructure in Support of Research: A New Imperative*, OCI 04-38712, $41.1M, 7/06-8/08; *ETF Early Operations-NCSA*, OCI 04-51538, $1.9M, 3/05-9/06; *ETF Grid Infrastructure Group (U of Chicago lead)*, OCI 05-03697, $14.1M, 9/05-7/11; *TeraGrid Resource Partner-NCSA*, OCI 05-04064, $4.2M, 9/05-7/11; *Empowering the TeraGrid Science and Engineering Communities*, OCI 05-25308, $17.8M, 10/07-7/11; *Critical Services for Cyberinfrastructure: Accounting, Authentication, Authorization and Accountability Services (U of Chicago lead)*, OCI 07-42145, $479k, 10/07-9/09.

Phil Andrews is the first Project Director of the National Institute for Computational Sciences, the home of the NSF Track 2B award for a petascale computer system, where he is responsible for overall management and technical leadership. He is the author of approximately 40 papers on grid and data intensive computing, documentation and visualization techniques, theoretical plasma physics, and nonlinear dynamics. He is on the TeraGrid Executive Steering and the EGEE External Advisory and other committees. Prior to NICS, he was Director of High End Computing Technologies at the San Diego Supercomputer Center, where he instantiated the first production wide-area parallel global filesystem, GPFS-WAN, and was the SDSC PI on the ETF Grid Infrastructure Group award.

P. Andrews: *High Performance Computing System Acquisition: Towards a Petascale Computing Environment for Science And Engineering*, NSF, $64M, 10/07-9/12; *TeraGrid GIG Subaward – ASTA, PM and QA/CUE*, $504k, 08/08-07/09; *ETF Grid Infrastructure Group (U of Chicago lead)*, OCI 05-03697, $7.7M, 08/05-07/09.

Jay Boisseau is the director of the Texas Advanced Computing Center. In nine years, he has taken the center from a small facility to a premier supercomputing center offering some of the most powerful HPC and visualization capabilities for open science in the world. He is the PI of TACC's TeraGrid activities, is the PI and Project Director for NSF's inaugural 'Path to Petascale' HPC system (Ranger), and is the PI for TACC's role in the DoD Programming Environment & Training program. He initiated TACC's Scientific Computing Curriculum, which now offers five academic classes for graduate and undergraduate students. Under his guidance, TACC has also developed R&D programs, producing widely used software (GotoBLAS, MyCluster, TeraGrid User Portal, etc.) and EOT programs that promote interest and participation in computational disciplines. Prior to TACC, he was the Associate Director for Scientific Computing at the San Diego Supercomputer Center, where he created the Strategic Applications Collaboration program and led development of the first grid user portal for NSF users.

J. Boisseau: *Enhancing the Capabilities, Scope, and Impact of the Extensible Terascale Facility,* ACI 03-38629, $3.2M, 10/03-09/06; *TeraGrid: Early Operations*, SCI-0451543, $743k, 03/05-02/06; *TeraGrid: Resource Partners,* OCI 05-04077, $10M, 04/05–02/10; *World-Class Science Through World Leadership in HPC*, OCI-06-22780, $59M, 10/06-09/11; ETF Grid Infrastructure Group (U of Chicago lead), OCI 05-03697, $7.7M, 08/05-07/09.

Ralph Roskies is Professor of Physics at the University of Pittsburgh and a founder and Co-Scientific Director of the Pittsburgh Supercomputing Center (PSC). He is the author of over 60 papers in theoretical elementary particle physics. As PSC Scientific Director, Roskies oversees operations, plans its future course, and concerns himself with its scientific impact. The PSC has pioneered developments in filesystems, heterogeneous computing, parallel algorithms and scientific visualization, and is renowned for outstanding user support. He has served as advisor to and as reviewer of a large number of U.S. and international supercomputing centers. Roskies' pivotal role in developing and implementing the NSF allocation process has given him a very broad overview of leading computational science and close ties to its most prominent practitioners.

R. Roskies: *ExTENCI: Extending Science Through Enhanced National Cyberinfrastructure (U of Florida lead),*NSF, $382k; 5/10-3/12; *Planning for XSEDE: the eXtreme Science and Engineering Discovery Environment (Illinois lead),* NSF OCI 09-41686, $501,000, 4/09- 7/10; *TeraGrid Extension: Bridging to XD (U of Chicago lead),* NSF OCI 09-32251 $4.6M, 4/10-3/11; *TeraGrid Resource Partners,* NSF, SCI 04-56541, $52M , 8/05-3/11; *ETF Grid Infrastructure Group: Providing System Management and Integration for the TeraGrid (U of Chicago lead),* NSF, SCI 05-03697, $4.7M, 8/05-3/11; *Terascale Computing System (NETL Support),* CSA OSI 05-08665, NSF, $5.1M, 10/04-9/09; *Terascale Computing System*, ACI 03-07136, NSF/ACIR, $63M, 10/00-9/05.